(56)

Modeling Water Chemistry and Electrochemical Corrosion Potential in Boiling Water Reactors

by

David J. Grover

B.S. Mechanical Engineering
University of Maine

SUBMITTED TO THE DEPARTMENT OF NUCLEAR ENGINEERING IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

MASTER OF SCIENCE IN NUCLEAR ENGINEERING
AT THE
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

September 1996

Signature of Author:_____
Department of Nuclear Engineering
August 14,1996

Certified By:_____
R. G. Ballinger
Associate Professor of Nuclear Engineering
Thesis Supervisor

Certified By:_____
R. M. Latanison
Professor of Materials Science and Engineering
Thesis Reader

Accepted By:_____
J. P. Freidberg
Professor of Nuclear Engineering
Chairman, Committee for Graduate Students

Modeling Water Chemistry and Electrochemical Corrosion Potential in Boiling Water Reactors

by

David J. Grover

Submitted to the Department of Nuclear Engineering
on August 1996 in partial fulfillment of the
Requirements for the Degree of
Master of Science in Nuclear Engineering

Abstract

Computer Simulations of a two typical Boiling Water Reactors (BWR), a BWR-3 and a BWR-4, primary coolant chemistry have been completed with particular attention to O_2, H_2, and H_2O_2 concentrations. Electrochemical corrosion potentials (ECP) values have also been calculated along the coolant path length using the calculated chemical concentrations as well as fluid velocity. The simulations run were both for normal water chemistry (NWC) operating conditions as well as hydrogen water chemistry (HWC) operating conditions.

For this project the MIT water radiolysis code, RADIation Chemistry Analysis Loop Code (RADICAL), was modified to calculate chemical species concentrations as the fluid passes through variable cross-sectional area regions in the BWR. This modification allows detailed determination of velocity along the flow path, which allows for more accurate ECP calculations.

The simulation results show that hydrogen injection decreases the concentrations of both oxygen and hydrogen peroxide through-out the primary system. The simulations of a water sample taken from the recirculation line agree well with in-plant measurements of the same, especially well for the BWR-4 where the results are nearly identical for injection levels corresponding to oxygen concentrations above 1 ppb.

Parametric studies were conducted to test the effect of thermal hydraulic parameters on the results with power, radiation dose rates, and hydraulic diameters for components with diameters less than 30 cm having the greatest effect. In addition studies were conducted to map the effect operating in the allowable ranges of power and flow has on ECP. The results indicate some permissible power-flow combinations should be avoided to minimize plant ECP.

Thesis Supervisor: Ronald Ballinger
Title: Associate Professor of Nuclear Engineering and Materials Science and Engineering

Acknowledgements

Recognition and thanks are due Professor Ronald Ballinger for his guidance and his support over the course of this project. I am very grateful for all the assistance and advice he has offered me not only on this project but also on my internship. Acknowledgment and thanks to Dr. John Chun for his help in working with the RADICAL code and his many insights on water chemistry.

I deeply appreciate the opportunity the Defense Nuclear Facilities Safety Board gave me to attend graduate school at the Massachusetts Institute of Technology.

Finally I would like to thank my family, especially my mother, Carol, for her years of support and encouragement when I decided to return to college after completing my apprenticeship at the Portsmouth Naval Shipyard.

Table of Contents

List of Figures

List of Tables

1. INTRODUCTION

Environmentally assisted cracking (EAC) of structural materials in boiling water reactors (BWR's) has been a major concern in the power industry for some time. The specific type of EAC of concern in BWR's is intergranular stress corrosion cracking (IGSCC). Stress corrosion cracking requires three conditions to occur [Jones 1992] (1) a susceptible material, (2) tensile stress, and (3) a corrosive environment. Eliminating any one of these three conditions will eliminate IGSCC. This in turn extends the life of primary system components, extending the useful life of the power plant.

While the environment within cracks is the controlling environmental factor in crack propagation, the general water chemistry is a significant contributer by acting as a boundary condition to the local environment. In BWRs, the radiolysis of coolant water by gamma and neutron radiation results in dissolved oxygen concentrations of 150 to 300 ppb under normal water chemistry conditions. Experimental studies have shown that reducing the electrochemical corrosion potential (ECP) to below -230 mV, referenced to a standard hydrogen electrode (SHE), corresponding to a dissolved oxygen concentration of less than 20 ppb will effectively protect the system against IGSCC [Cowan 1986].

One method of reducing dissolved oxygen concentration is to inject hydrogen into the feedwater supply. However, excessive hydrogen reacts not only with oxygen but with nitrogen, including radioactive nitrogen 16. These nitrogen compounds are released into the main steam lines and can increase the radiation levels in the manned operating areas of the plant to unacceptable levels. To determine the optimal level of hydrogen addition an analytical model of water chemistry is necessary, as in-plant monitoring of water chemistry is generally not sufficient because the chemistry changes in the sampling lines,

once removed from the radiation levels present in the primary system. The primary cause for this change being the rapid decomposition of hydrogen peroxide at the operating water temperature.

MIT radiolysis modeling was begun in 1988 by Simonson with the MITIRAD code [Simonson 1988]. The initial code was used to simulate radiolysis in high level waste packages in underground repositories. In 1990 this model was expanded by Chun to simulate BWRs and renamed RADICAL, RADIation Chemistry Analysis Loop code [Chun 1990]. This FORTRAN code models the following processes: radiolysis of water into chemical species, convection of the fluid, mass transport between gas and liquid phases, chemical generation of species, and chemical annihilation of the species. In addition, a sensitivity model was included to determine the relative importance of various input parameters to output concentrations. In 1993, improved thermal hydraulic models were added [Chun 1993]. For this thesis the model is further expanded and reformulated to allow for variable cross-sectional flow regions which better represent fluid velocities in the primary system. Also, improved ECP correlations have been added which take into account not only oxygen concentrations but also liquid velocity, hydrogen peroxide concentration, and hydrogen concentration.

The RADICAL model, as it has been modified, takes as input chemical reaction data, g-values, radiation dose rates, and thermal hydraulic parameters. The concentrations are then calculated using a differential equation solver. The model is very flexible, and can allow chemical reactions in addition to water reactions by adding them to the chemical reaction matrix. RADICAL has also been used to model systems other than BWR water chemistry, including the BWR Corrosion Chemistry Loop (BCCL) and the Irradiation Assisted Stress Corrosion Cracking Loop (IASCC) at the MIT research reactor.

The current BWR model is an approximation which attempts to best describe water chemistry given the current available input. The model has grown more complex since the 1993 version and will continue to increase in complexity as more detailed input data becomes available. Included in this thesis are parametric studies used to determine the degree of accuracy needed to model thermal hydraulic parameters and radiation dose rate profiles while still allowing the model to be run in 'real time' using a desktop PC, the current version running on Powerstation FORTRAN 1.0 for Windows NT, a FORTRAN 77 compiler.

2. Background

Environmentally assisted cracking (EAC) of structural materials in boiling water reactors (BWR's) has been a major concern in the power industry for some time. The specific type of EAC of concern in BWR's is intergranular stress corrosion cracking (IGSCC). Stress corrosion cracking requires three conditions to occur [Jones 1992]:

1. A susceptible material. The reactor vessel components are typically fabricated from austenitic stainless steel which is susceptible to sensitization and IGSCC.
2. A tensile stress. The primary system of a Boiling Water Reactor (BWR) has an operating pressure of approximately 7.2 MPa. This results in the reactor vessel and associated piping being in a state of tensile stress as well having residual stresses from vessel assembly and welding.
3. A corrosive environment. Radiolysis results in an oxygenated coolant, experimental measurements have shown oxygen levels of approximately 200 ppb in the recirculation line [Ruiz 1989]. In addition the operating temperature of a BWR is about 300 °C.

Eliminating any one of these three conditions will eliminate IGSCC. This in turn extends the life of primary system components, extending the useful life of the power plant.

While the water chemistry within cracks is a factor in crack propagation, the general water chemistry is a significant contributer by acting as a boundary

condition to the local environment. In BWRs, the radiolysis of coolant water by gamma and neutron radiation results in dissolved oxygen concentrations of 150 to 300 ppb under normal water chemistry conditions. Experimental studies have shown that reducing the electro-chemical corrosion potential (ECP) to below -230 mV, referenced to a standard hydrogen electrode (SHE), corresponding to a dissolved oxygen concentration of less than 10 ppb will effectively eliminate IGSCC [Cowan 1986].

One method of reducing dissolved oxygen concentration is to inject hydrogen into the feedwater supply. To determine the optimal level of hydrogen addition an analytical model of water chemistry is necessary, as in plant monitoring of water chemistry is generally not sufficient because the chemistry alters in the sampling lines once removed from the radiation levels present in the primary system

2.1. Previous Work in Water Chemistry Modeling

Numerous water chemistry models have been developed in the past 25 years and are listed below in Table 2.1.

Current models for radiolysis are embodied in the computer codes SIMFONY [Ibe, et al. 1986,1987, 1995], FACSIMILE [Ruiz, et al. 1989; Romeo et al. 1995], RADIOCHEM [Yeh and Macdonald 1995], and RADICAL [Chun 1990, 1993] are used to model water chemistry in BWRs. Most of the results are qualitative in nature as most parameters are not accurately known. In addition there is lack of

plant data for comparision with the only data available being oxygen and hydrogen concentrations for samples taken from the recirculation line.

Table 2.1 Water Chemistry Models [Ibe and Uchida 1985]

Program Name	**Publication Information**	**Principal Mathematical Method**
WR20	Schmidt (1970)	5-th order Adams Bashforth Formulas
CHEK	Burns and Moore (1976)	Backward differentiation Formulas (BDF)
FACSIMILE	Burns and Moore (1976)	BDF combined with nonlinear algebraic equations Sparse matrix routine
MAKSIMA	Boyd et al. (1979)	BDF with sparse matrix routine
AQUARY	Ibe and Uchida (1982)	Iterative procedures with BDF for a set of differential-integral equations
SIMFONY	Ibe and Uchida (1983)	Extension of Aquary BDF
RADIOLYSIS MODEL	Takagi, et al. (1988)	BDF
RADICAL	Chun (1990, 1993)	BDF combined with nonlinear algebraic equations
RADIOCHEM	Yeh and Macdonald (1995)	BDF

2.2. G-Values

The quantity of chemical species produced by radiolysis is quantitatively described by g-values which give the number of molecules produced per 100 eV of energy deposited in a media by radiation. Each type of radiation has a differing effect on the media resulting in a g-value for each combination of radiation and produced chemical species. While g-values for stable species, O_2, H_2, and H_2O_2, can be directly measured. The g-values for short lived chemical radicals, e^-_{aq}, H^+, H, OH, O, O_2^-, and HO_2, must be calculated using a mass

balance. Adding to the difficulty of determining these parameters is a temperature dependence which differs between gamma and neutron radiation [Ruiz 1989, McCracken 1990]. Of the published sets of g-values, Table 2.2, The model currently uses the Burns values, column A, for neutron dose [1976], and the Kent and Sims gamma dose values, column E [1992] with the OH g-values modified to provide a redox balance and the others modified slightly to provide a stoichiometricly balanced set.

Table 2.2 Summary of Neutron and Gamma Radiation G-values [Ibe 1989]

	G-Value (#/100eV)							
	Neutron			Gamma				
Species	A	B	C	A	B	C	D	E
e^-_{aq}	0.93	0.4	0.37	2.7	0.4	2.8	4.15	3.69
H^+	0.93	0.4	0.37	2.7	0.4	2.8	4.15	3.69
H	0.5	0.3	0.36	0.62	0.3	0.55	1.08	0.68
H_2	0.88	2.0	1.2	0.43	2.0	0.45	0.62	0.72
H_2O_2	0.99		0.97	0.62		0.72	1.25	0.28
HO_2	0.04		0.17	0.03				
OH	1.09	0.7	0.46	2.9	0.7	2.7	3.97	4.64
O		2.0			2.0			

A: Burns' values for 25°C [1976]
B: Burns' values for high temperatures, 300-410°C [1976].
C: Christensen's values based on Forsmark-2 [1982].
D: Elliot's values for high temperature, 300°C [Elliot, Chenier 1990]
E: Kent and Sims' values for high temperature, 270°C [1992]

2.3. Chemical Reactions

Once chemical species are produced by radiolysis chemical reactions need to be specified to govern their consequent interactions. This is controlled within the model by chemical reaction sets. For coding purposes reaction sets are composed of three parts (1) a symbolic representation of the chemical reaction occurring, (2) the rate constant which governs the speed of the reaction, and (3) the activation energy which determines the difficulty of initiating the reaction. Modeling the water chemistry relies on knowing these three quantities accurately. However, as is the case with g-values several reaction sets are available. Current sets available are those listed by Simonsen [1988], as well as those used by Ibe [1986], Ruiz [1993],the set currently used, and Romeo [1995].

2.4. Operating Parameters

For each BWR there is a set of operating parameters unique to that plant. The first group of parameters are the radiation doserates that directly produce radiolytic species. Previously doserates were estimated for the reactor core using typical values from computer codes. Doserates in other regions were calculated from these core regions using shielding theory for the attenuation by vessel components and the primary coolant. The current RADICAL model uses results of Monte Carlo calculations which are scaled to each plant based on power densities [Romeo 1995].

The thermal-hydraulic parameters which characterize each region of the primary coolant path are pressure, temperature, power, mass flow rate, fluid properties,

flow geometry and hydraulic diameters. For this Thesis these parameters have been calculated using data from Romeo [1995]. In addition flow geometry for jet pumps and steam separators have been obtained from the Pilgrim Nuclear Station Final Safety Analysis Report (SAR). Calculation of these parameters is discussed in Appendix A, Section 4.

2.5. Previous Work in ECP Modeling

Experimental studies have shown that reducing the ECP to below -230 mV (SHE) will effectively eliminate intergranular stress corrosion cracking in stainless steel. Studies showed -230 mV SHE corresponded to an approximate oxygen concentration of 20 ppb [Cowan 1986]. This led to the development of water chemistry models to predict chemical species concentrations. To determine the ECP related to the predicted concentrations an ECP correlation was developed as a function of oxygen concentration only [Lin et.al. 1992]. However, the corrosive potential is not only due to the reduction of oxygen and oxidation of stainless steel. Hydrogen peroxide is also reduced and hydrogen is oxidized. In addition flow velocity has an effect on concentration potentials. To account for these addition parameters Macdonald used a mixed potential model to calculate ECP [1992]. Lin has also developed a mixed potential ECP correlation which is currently used by RADICAL to calculate ECP [1993] and is described in detail in Section 5.

3. Theoretical Modeling of Water Chemistry

The concentration of chemical species in the modelL are calculated using mass balance equations for each species. These equations are derived for two-phase flow through a differential control volume. The differential equations represent the concentration as a function of position, dC/dx.

3.1. Concentration Equation Derivation

To model the dissolution and recombination of water in boiling water reactors the following mechanisms must be accounted for:

- Generation due to radiolysis by neutron and gamma radiation,
- Generation due to chemical reactions,
- Annihilation due to chemical reactions,
- Fluid convection,
- Mass transfer of species between vapor and liquid in two-phase flow.

The differential equations for the concentration of chemical species can be derived with respect to either time or space, with the two related by the fluid velocity. However, in two-phase flow the vapor and liquid velocities are unequal resulting in slip between the two phases. If the differential equations are taken with respect to time, the respective masses of the two phases will be in different locations at the same time interval, resulting in more complex differential equations. As a result, spatially based, with respect to position, derivatives are

chosen for modeling. To solve for the concentration of chemical species in the fluid, a mass balance is developed for the control volume shown in **Figure 3-1**.

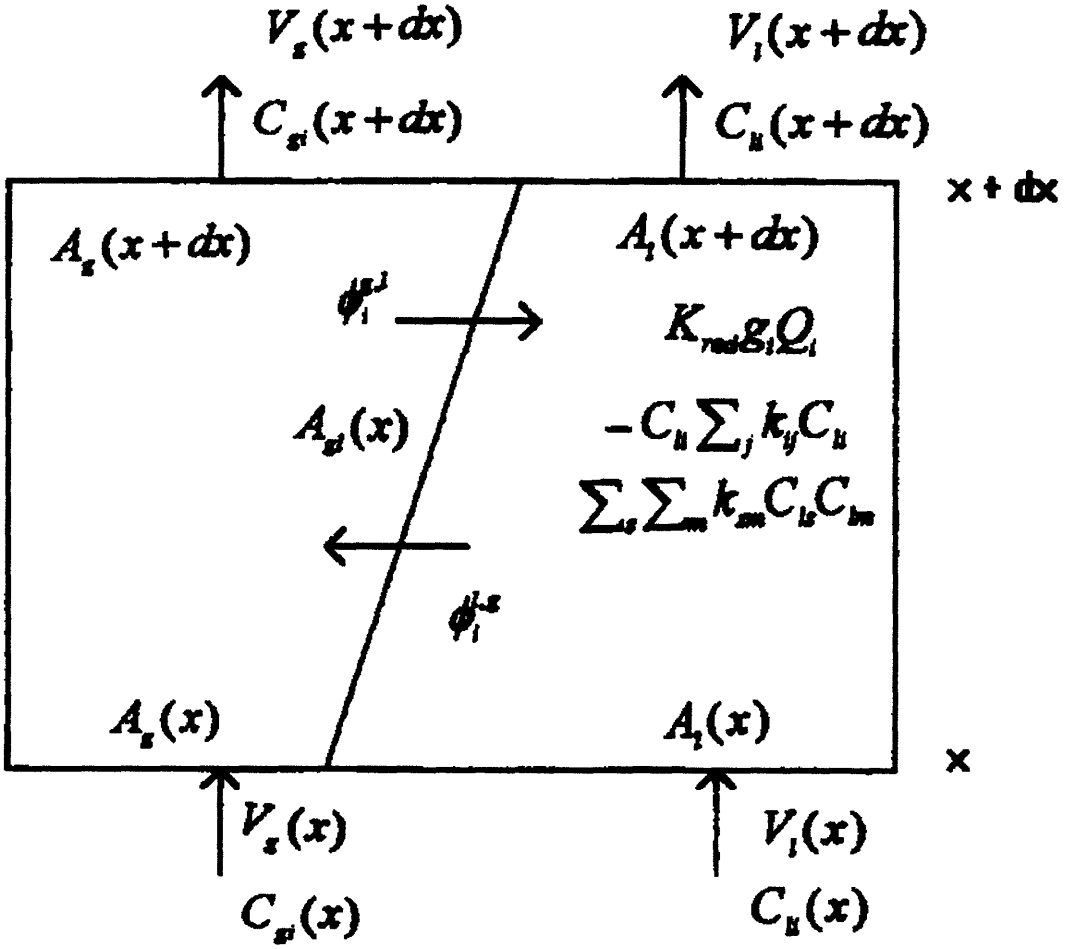

Figure 3.1 Differential Control Volume Element for a Two-Phase Fluid [Chun 1990]

The mass balance for the liquid phase of the differential control volume is given by the following equation.

$$\frac{d\left[C_{li}A_l(x)dx\right]}{dt} = A_l(x)dx\left[K_{rad}g_iQ_i + \sum_s\sum_m k_{sm}C_{ls}C_{lm} - C_{li}\sum_j k_{ij}C_{lj}\right]$$
$$+V_l(x)A_l(x)C_{li}(x) - V_l(x+dx)A_l(x+dx)C_{li}(x+dx) \qquad (3.1)$$
$$+A_{gl}(x)\left(\phi_i^{g,l} - \phi_i^{l,g}\right) = 0$$

Where: C :Concentration of the given species (mol/l)
A :cross-sectional area (cm^2)
V :fluid velocity
K_{rad} :conversion factor for g-values (from #/100eV to mol/l-Rad)
g :g-value of the given species (#/100eV)
Q :dose rate (Rad/s)
ϕ :concentration flux across the gas-liquid interface
g :in subscript refers to gas phase
l :in subscript refers to liquid phase
gl, :in subscript refers to the gas-liquid interface, in superscript it refers to the direction of transfer, i.e. gas to liquid
i :refers to the i-th chemical species
j :refers to the j-th species which reacts with the i-th species
m,s :refers to alternate species reacting together to form the i-th species

Similarly, the mass balance for the gas phase is given by the following equation:

$$\frac{d\left[C_{gi}A_g(x)dx\right]}{dt} = V_g(x)A_g(x)C_{gi}(x) - V_g(x+dx)A_g(x+dx)C_{gi}(x+dx) + A_{gl}(x)\left(\phi_i^{l,g} - \phi_i^{g,l}\right) = 0 \tag{3.2}$$

The (x+dx) terms are expanded using Taylor series.

$$\begin{aligned} &C_i^l(x+dx)V_l(x+dx)A_l(x+dx) \cong \\ &\left[C_i^l(x) + \frac{\partial C_i^l}{\partial x}dx\right]\left[V_l(x) + \frac{\partial V_l}{\partial x}dx\right]\left[A_l(x) + \frac{\partial A_l}{\partial x}dx\right] \cong \\ &C_i^l(x)V_l(x)A_l(x) + C_i^l(x)V_l(x)\frac{\partial A_l}{\partial x}dx + C_i^l(x)A_l(x)\frac{\partial V_l}{\partial x}dx + \\ &V_l(x)A_l(x)\frac{\partial C_i^l}{\partial x}dx \end{aligned} \tag{3.3}$$

In this expression second and higher order terms of the Taylor expansion have been neglected. Also terms containing multiples of dx, i.e. dx^2, have been omitted as these terms are negligible compared to the others.

In addition the relationship between the cross-sectional area of the phases, the total cross-sectional area and the void fraction must be characterized to obtain the final concentration differential equations.

3.2. Cross-Sectional Area and Void Fraction Relationships

Cross-sectional area and void fraction relationships are used to eliminate the liquid and vapor cross-sectional areas which cannot be adequately characterized any other way. for this thesis the model has been enhanced from the original RADICAL model to allow for the use of variable total cross-sectional area flow regions.

The void fraction is the fraction of volume or area which is occupied by the vapor phase of a two-phase fluid. Therefore the area occupied by the vapor phase can be represented as the product of the void fraction and the total cross-sectional area, Eq. 3.4. Similarly the area occupied by the liquid phases can be represented by the product of the total cross-sectional area and the compliment of the void fraction, Eq. 3.6. Differentiating these equations, assuming total area to be variable yields Eq. 3.5 and Eq. 3.7.

$$A_g(x) = \alpha(x) A_T(x) \tag{3.4}$$

$$\frac{\partial A_g(x)}{\partial x} = A_T(x)\frac{\partial \alpha(x)}{\partial x} + \alpha(x)\frac{\partial A_T(x)}{\partial x} \tag{3.5}$$

$$A_l(x) = [1-\alpha(x)] A_T(x) \tag{3.6}$$

$$\frac{\partial A_l(x)}{\partial x} = -A_T(x)\frac{\partial \alpha(x)}{\partial x} + [1-\alpha(x)]\frac{\partial A_T(x)}{\partial x} \tag{3.7}$$

Where the subscript T represents the total cross-sectional area.

3.3. Chemical Reactions

Chemical reactions are represented in EQ. 3.1 by the relationship:

$$\sum_s \sum_m k_{sm} C_{ls} C_{lm} - C_{li} \sum_j k_{ij} C_{lj}$$ [Ibe 1985]

The first term represents the production of a chemical species by the interaction of all species which can form this species. The second term represents the annihilation of a chemical species by interactions with all other species with which it can react. This is repeated for all chemical species.

For a chemical reaction:

$$A + B \rightarrow C + D \tag{3.9}$$

The kinetics for the generation of species C is given by:

$$\frac{d[C]}{dt} = k[A][B] \tag{3.10}$$

The kinetics for the annihilation of species A is given by:

$$\frac{d[A]}{dt} = -k[A][B] \tag{3.11}$$

These equations are identical except for the sign, depending on whether it is a reactant or a product. Because of this relationship the model in RADICAL uses a single coefficient, KOEF, to keep track of both generation and annihilation of chemical species [Simonson 1988]. This new reaction solving method is given by the following relationship:

$$\sum_{j=1}^{NRX} KOEF_{ji} k_j \prod_{m=1}^{3} C_{mi}^{l}(x) \tag{3.12}$$

The product is carried out over all reactions in a reaction set matrix with the species being summed over all the reactions. The reactions in a reaction matrix consist of the standard chemical reaction equation coupled with the reaction rate constant and activation energy. The current reaction set being used in the model is given in **Table 3.1**

Table 3.1 Chemical Reaction Sets

RX Name	Reactants		Products			Reaction Rates	Activation Energy
f3	e-	H2O	>H	OH-		1.6e1	12.55
f4	e-	H+	>H			3.5e+11	0.e0
f5	e-	OH	>OH-			2.0e+10	12.55
f6	e-	H2O2	>OH	OH-		1.3e+11	0.e0
f7	H	H	>H2			8.5e10	0.e0
f8	e-	HO2	>HO2-			2.0e10	12.55
f9	e-	O2	>O2-			2.6e11	0.e0
f10	e-	e-	>OH-	OH-	H2	5.e9	12.55
f11	OH	OH	>H2O2			1.7e10	0.e0
f12	H	OH-	>e-	H2O		2.0e7	18.83
f13	H	e-	>H2	OH-		2.5e10	12.55
f14	HO2-	e-	>OH	OH-	OH-	3.5e9	12.55
f15	H	OH	>H2O			5.5e10	0.e0
f16	H2	OH	>H	H2O		4.e7	18.0163
r16	H	H2O	>OH		H2	1.042e-4	85.1695
f17	H	O2	>HO2			8.6e10	0.e0
f18	H	HO2	>H2O2			2.e10	12.55
f19	H	O2-	>HO2-			2.e10	12.55
f20	O2-	e-	>HO2-	OH-		1.3e8	18.83
f21	H	H2O2	>OH	H2O		9.e7	16.61466
f22	H2O2	OH	>H2O	HO2		3.e7	13.01224
f23	HO2	OH	>O2	H2O		8.6e10	0.e0
f24	H2O2	OH-	>HO2-		H2O	1.8e10	12.55
r24	HO2-		>H2O2		OH-	5.7e5	18.83
f25	HO2	HO2	>O2	H2O2		8.5e5	22.82372
f26	HO2		>H+	O2-		2.565e4	12.55
r26	O2-	H+	>HO2			5.e10	12.55
f27	HO2	O2-	>HO2-	O2		5.e9	0.e0
f29	H+	OH-	>H2O			1.44e11	12.55
r29			>H+	OH-		0.79242	12.55
f30	OH	O2-	>O2	OH-		8.6e10	0.e0
tif	1/2O2	1/2O2	>O2			1.e15	0.e0
W32	H2O2		>OH	OH		2.00E-03	0.0
SS	H2O2		>1/2O2		H2O	0.124	0.0

The reaction rates are given for a reference temperature of 25°C and adjusted to reactor operating conditions, approximately 300°C using an Arrhenius law.

3.4. Radiolysis

Radiolysis is the production of chemical species by ionizing radiation. When water, H_2O, is irradiated by gamma rays and fast neutrons it will dissociate into various radicals, ionized, and stable chemical species. For the purposes of this thesis only water is considered to undergo radiolysis with the following species being produced:

$$H_2O \rightarrow e_{aq}^-, H^+, H, OH, O, HO_2, H_2, H_2O_2$$

The rate of production of these species is proportional to the amount of energy deposited in the medium by the radiation, i.e. dose. The number of molecules produced per 100 eV is defined as the g-value of the radiation and is determined experimentally for each type of radiation. These g-values are converted to moles per liter per Rad for use in the model. The production is the product of the modified g-value and the dose in the control volume given by the relation from EQ. 3.1:

$$K_{rad} g_i Q_i$$

The g-values used in the liquid phase are given in **Table 3.2**. Radiolysis is not considered in the vapor phase as the density of this phase is so small that the interaction between radiation and water vapor produces negligible quantities of chemical species.

Table 3.2 G-Values for High Temperature Water

Chemical Species	G-Value #/100eV	
	Gamma	Neutron
e^-_{aq}	3.76	0.93
H^+	3.76	0.93
H	0.7	0.5
OH	5.5	1.09
HO_2	0.0	0.04
H_2	0.8	0.88
H_2O_2	0.28	0.99

3.5. Convection

Convection is represented in Eq. (3.1) and Eq. (3.2) by the following relationship with respect to liquid or gas phase respectively:

$$V_{g/l}(x)A_{l/g}(x)C_{g/li}(x) - V_{g/l}(x+dx)A_{g/l}(x+dx)C_{g/li}(x+dx)$$

This relationship represents the time dependent change of concentration across the differential volume as a function of concentration, velocity, and flow-phase cross-sectional area gradients. In the previous version of the RADICAL model the area gradients existed only in two-phase flow and were functions of void fraction only. For this thesis the fluid-phase cross-sectional area gradient is a function of both void fraction and total cross-sectional area by incorporating the equations derived in Section 3.2. Now changes in physical dimensions, i.e. pipe diameters, are factors in convection for both single-phase and two-phase flow.

3.6. Mass Transfer Between Liquid and Vapor Phases

The flux of chemical species between the gas and liquid phases are represented in Eqs. 3.1 and 3.2 by the following relationship:

$$A_{gl}(x)\left(\phi_i^{g,l} - \phi_i^{l,g}\right)$$

This is the difference between the flux into the phase minus the flux out of the phase multiplied by the boundary surface area A_{gl}. These terms are represented by the following equations [Ibe, 1986]:

$$A_{gl}(x) = \frac{6\alpha}{d_b} A_T(x)dx \qquad (3.13)$$

$$\phi_i^{g,l} = k_i^{g,l}\left(C_{li} - aC_{li}\right) \qquad (3.14)$$

$$\phi_i^{l,g} = k_t^{l,g}\left(C_{gi} - bC_{gi}\right) \tag{3.15}$$

The constant, 6, divided by the bubble diameter is considered a constant at a given pressure and is incorporated into a new constant along with the rate constant and the constants a and b. These constants are proportionality constants to describe the concentration gradient between the bulk fluid and the fluid at the bubble surface. This new constant (μ) is given by the following expression:

$$\mu_i^{l,g} = \frac{6k_t^{l,g}}{d_b}(1-\alpha) \tag{3.16}$$

$$\mu_i^{g,l} = \frac{6k_t^{g,l}}{d_b}(1-\beta) \tag{3.17}$$

These are referred to as the mass transfer constants, with the values used in the RADICAL model given in **Table 3.3**

Table 3.3 Mass Transfer Constant Values for Use in Radiolysis Models [Ibe 1985]

	H2	O2
$\mu_i^{l,g}$	30	23
$\mu_i^{g,l}$	9.9	12.4

3.7. Concentration Equations

Incorporating the relationships from Sections 3.2 through 3.6 into EQs. 3.1 give the following differential equation for the concentration in the liquid phase:

$$\frac{dC_{li}(x)}{dx} = \frac{1}{V_l(x)} \left\{ \begin{array}{l} \left[K_{rad} g_i Q_r + \sum_{j=1}^{NRX} KOEF_{ji} k_j \prod_{m=1}^{3} C_{mi}^{l}(x) \right] \\ -C_{li}(x) \frac{\partial V_l}{\partial x} + \left(\mu_i^{g,l} C_{gi}(x) - \mu_i^{l,g} C_{li}(x) \right) \frac{\alpha(x)}{1-\alpha(x)} \\ + \frac{C_{li}(x) V_l(x)}{1-\alpha(x)} \frac{\partial \alpha(x)}{\partial x} + \frac{C_{li}(x) V_l(x)}{A_T(x)} \frac{\partial A_T(x)}{\partial x} \end{array} \right\} \tag{3.18}$$

Similarly, the differential equation for the gas phase is:

$$\frac{dC_{gi}(x)}{dx} = \frac{-1}{V_l(x)} \left\{ \begin{array}{l} C_{gi}(x) \frac{\partial V_g}{\partial x} + \left(\mu_i^{l,g} C_{li}(x) - \mu_i^{g,l} C_{gi}(x) \right) \\ + \frac{C_{gi}(x) V_g(x)}{\alpha(x)} \frac{\partial \alpha}{\partial x} - \frac{C_{gi}(x) V_g(x)}{A_T(x)} \frac{\partial A_T}{\partial x} \end{array} \right\} \tag{3.19}$$

Again radiolysis and chemical reactions are not considered in the gas phase. This is due to these reactions being dependent on the density of the fluid, which is approximately five percent of the density of the liquid phase. As a result the contributions of radiolysis in the vapor will be negligible. These two equations describe the concentration of various species produced by radiolysis and associated chemical reactions.

3.8. Void Fraction and Velocity Slip

In addition to these equations thermal-hydraulics must be used to describe the properties of the fluid in the boiling region of the system. This is done using one of two correlations, either Bankoff's or the Chexal-Lellouche [Chun 1993], depending on which input parameters are available. The selection of a correlation based on available data is discussed in Appedix A.

3.8.1. Bankoff Correlations

Primarily the void fraction and fluid velocities must be calculated, which is accomplished using Bankoff's correlation's [Todreas 1990]:

$$\alpha(x) = \frac{1}{C_0} \frac{1}{1 + \left(\frac{1 - \chi(x)}{\chi(x)} \right) \frac{\rho_v}{\rho_l}} \tag{3.20}$$

$$\frac{1}{C_o} = 0.833 + 0.0001P(psi)$$

where: χ :is the fluid quality
ρ :is the density of the phases

The quality of the fluid is a function of the heat input in the reactor core. [Ibe 1986]

$$\chi(x) = \begin{cases} 0, (x < x_b) \\ \frac{q_t}{2h_{fg}} - \frac{h_f - h_i}{h_{fg}} - \frac{q_t}{2h_{fg}} \cos\left(\frac{\pi x}{h_L} \right), (x \geq x_b) \end{cases} \tag{3.21}$$

$$q_t = h_f + \chi_e h_{fg} - h_i \tag{3.22}$$

$$x_b = \frac{h_L}{\pi} \cos^{-1}\left(\frac{h_i + \chi_e h_{fg} - h_f}{h_f + \chi_e h_{fg} - h_i} \right) \tag{3.23}$$

where i :is the value at the core inlet
e :is the value at the core outlet
L :is the core length
x_b :is the point in the reactor where boiling initiates
h :is the enthalpy

With the void fraction solved in terms of given operational parameters of the primary system, all that remains are expressions which give the gas and liquid velocities in terms of the operating parameters. This is done by defining the slip ratio, given by the following relation:

$$S(x) = \frac{V_g}{V_l} = \frac{1-\alpha(x)}{\frac{1}{C_0} - \alpha(x)} \tag{3.24}$$

The gas and liquid velocities are calculated from the fluid average velocity using the following equations:

$$\alpha\rho_g V_g + (1-\alpha)\rho_l V_l = \rho_l V_o \tag{3.25}$$

$$V_l = \frac{\rho_l V_o}{\rho_g \alpha S + \rho_l (1-\alpha)} \tag{3.26}$$

$$V_g = S V_l \tag{3.27}$$

The fluid average velocity is given by the definition of mass flow rate at the inlet point to the core:

$$V_o = \frac{\dot{m}}{A_T \rho_l} \tag{3.28}$$

These equations are sufficient to calculate the concentration of chemical species in the regions of the reactor containing two-phase flow.. These regions are the boiling channel of the core, the upper plenum and the 2-pahse region of the steam separator

3.8.2. Chexal-Lellouche Correlations

The Chexal Lellouche correlations [Chun 1993] use the following equations to represent fluid velocities.

$$V_l(x) = \frac{\dot{m}}{A_T(x)\rho_l(x)} \frac{(1-\chi(x))}{(1-\alpha(x))} \tag{3.29}$$

$$V_g(x) = \frac{\dot{m}\chi(x)}{A_T(x)\rho_g(x)\alpha(x)} \tag{3.30}$$

The thermodynamic quantities are calculated using the Chexal-Lellouche thermodynamic subroutines by inputting the initial temperature, pressure, and power input for the 2-phase region.

4. Computer Simulation of Water Chemistry

The radiolysis equations developed in Section 3 must be converted into a form suitable for computer calculation. During computations there will be **N** simultaneous differential equations to solve, one for each of the **N** chemical species being considered.

To solve these equations a standardized non-linear differential equation solver, LSODE, is used by RADICAL. LSODE was developed by Dr. Hindmarsh at Lawrence Livermore National Laboratory [Hindmarsh, 1983]. LSODE is used as an external subroutine with parameters calculated by RADICAL, input into LSODE, with LSODE returning results to the RADICAL code.

4.1. Computational Methodology of RADICAL

RADICAL reads input parameters for the system configuration necessary to complete the radiolysis calculations. The variables in the differential equations are then calculated and placed into an external subroutine, FRO, prepared by RADICAL to be passed to LSODE. Also passed to the subroutine FRO are the Jacobians for each of the equations.

RADICAL proceeds along the specified system calculating the concentrations at specified intervals. At each interval parameters and variables are updated, LSODE is called and new results are generated. This process continues until the system loop is completed. At this point the process can be repeated for a specifed number of loop cycles or until a convergence criteria is met.

4.2. Jacobian Derivation

As mentioned above the Jacobian of the equations is input to LSODE. LSODE can calculate this quantity internally, however a user-supplied Jacobian speeds calculation time.

The Jacobian of $\frac{\partial C_i}{\partial x}$ is defined as $\frac{\partial}{\partial C_k}\left(\frac{\partial C_i}{\partial x}\right)$ where the subscripts i and k span all chemical species. The Jacobian for the liquid phase differential equation 3.18 is

$$\frac{\partial}{\partial C_k}\left(\frac{dC_{li}(x)}{dx}\right) = \frac{1}{V_l(x)}\left\{\begin{array}{l}\left[\sum_{J=1}^{NRX} KOEF_{Ji} k_J \frac{\partial}{\partial C_k}\prod_{m=1}^{3} C_{ml}^{l}(x)\right] \\ -\frac{\partial C_{li}(x)}{\partial C_k}\frac{\partial V_l}{\partial x} + \frac{\partial}{\partial C_k}\left(\mu_i^{g,l} C_{gi}(x) - \mu_i^{l,g} C_{li}(x)\right)\frac{\alpha(x)}{1-\alpha(x)} \\ +\frac{\partial C_{li}(x)}{\partial C_k}\frac{C_{li}(x)V_l(x)}{1-\alpha(x)}\frac{\partial \alpha}{\partial x} + \frac{\partial C_{li}(x)}{\partial C_k}\frac{C_{li}(x)V_l(x)}{A_t(x)}\frac{\partial A_T(x)}{\partial x}\end{array}\right\} \quad (4.1)$$

$$\equiv Jac\left(C_{li}, C_k\right)$$

where

$$\frac{\partial C_{li}(x)}{\partial C_k} = \begin{cases} 0 & \text{if } i \neq k \\ \text{KOEF}_{ii} & \text{if } i = k \end{cases}$$

The Jacobian for the gas phase 3.19 is

$$\frac{\partial}{\partial C_k}\left(\frac{dC_{gi}(x)}{dx}\right) = \frac{-1}{V_l(x)}\left\{\begin{array}{l}\frac{\partial C_{gi}(x)}{\partial C_k}\frac{\partial V_g}{\partial x} + \frac{\partial}{\partial C_k}\left(\mu_i^{l,g} C_{li}(x) - \mu_i^{g,l} C_{gi}(x)\right) \\ +\frac{\partial C_{gi}(x)}{\partial C_k}\frac{V_g(x)}{\alpha(x)}\frac{\partial \alpha}{\partial x} - \frac{\partial C_{gi}(x)}{\partial C_k}\frac{V_g(x)}{A_T(x)}\frac{\partial A_T}{\partial x}\end{array}\right\} \quad (4.2)$$

5. Modeling of Electrochemical Corrosion Potential

The ECP model is based on the oxidation of the stainless steel, primarily iron, and hydrogen from radiolysis and feedwater injection. This is accomplished by the simultaneous reduction of oxygen and hydrogen peroxide.

5.1. Theoretical Modeling

The corrosion of BWR primary coolant systems is primarily due to half-cell reactions for the oxidation of hydrogen and stainless steel coupled with the reduction half-cell reactions for hydrogen peroxide and oxygen. The equilibrium potentials for each of these reactions are given by the Nernst equation:

$$E = E_0 + \frac{2.3RT}{nF}\log\frac{a_{oxid}}{a_{red}} \tag{5.1}$$

Where
E: half-cell potential
E_0: standard half-cell potential
R: gas constant
T: absolute temperature
n: number of electrons transferred in the reaction
F: Faraday constant
a_{oxid}: activity of the oxidized species
a_{red}: activity of the reduced species

The half-cell potential defines the potential at which the forward and reverse reactions are in equilibrium. Establishing these potentials gives the starting point for the development of the kinetics of the reactions.

A schematic of the Evan's diagram is shown in **Figure 5.1**

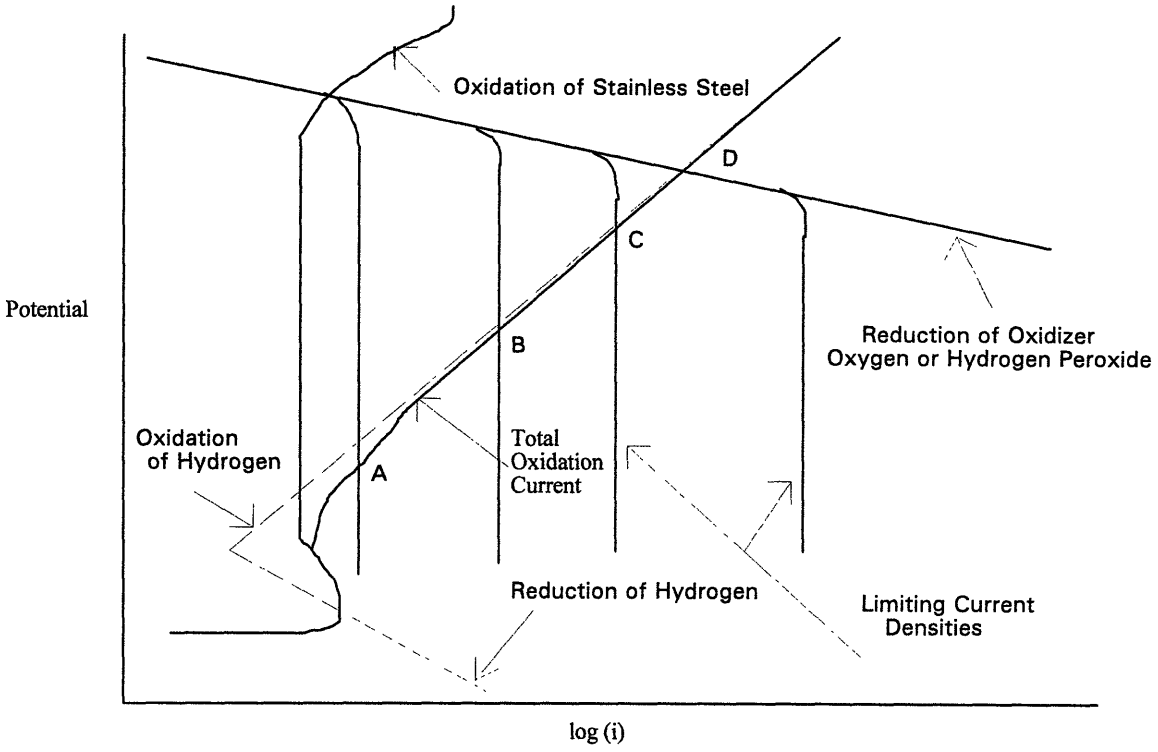

Figure 5.1 Schematic of Evan's Diagram for a Stainless Steel Surface

The kinetics of the reactions depend on activation and concentration polarization. Activation polarization is represented in Figure 5.1 as the oxidation and reduction lines for hydrogen, peroxide, and oxygen. The equation which represents these lines is:

$$E_\eta = E + \beta \log \frac{i_{a,c}}{i_0} \tag{5.2}$$

Where:

E_a: Activation potential
β: Tafel constant
i_a: current density, i.e. rate of oxidation or reduction
i_0: exchange current density, i.e. current density at the equilibrium potential

In addition to activation polarization there is also concentration polarization. This phenomena is characterized as a concentration gradient of H+ ions at the metal surface which depletes available hydrogen ions at the metal surface resulting in

a limiting reduction rate based on the diffusion and transport of hydrogen ions to the surface. This limiting current is given by the following equation:

$$i_L = \frac{DnFC}{\delta} \tag{5.3}$$

Where:
i_L: Limiting current density
D: Diffusion constant of the species
C: Concentration of the species in the bulk solution
δ: Boundary layer thickness

The multiple lines shown in Figure 5.1 represent this limiting current density for various degrees of fluid mixing. The higher limiting current densities representing a greater degree of mixing.

The stainless steel oxidation line is typical of a material with a passive region. The horizontal region at the lower potential of Figure 5.1 represent the Tafel constant region of the curve. The vertical portion represents the metal forming a protective passive layer which begins to breakdown at higher potential values. To determine the corrosion potential and associated corrosion rate, points A through D depending on the appropriate limiting current density, mixed potential theory is used. Using this the current densities for all oxidation reactions are summed forming the total oxidation current line in Figure 5.1. The same would be true for multiple reduction species.

To determine one corrosion potential for a BWR primary system would require that the parameters for Equations 3.1 - 3.3 be known for each species, as well as the fluid flow's effect on the limiting current density for all oxidizing species.

The determination of these parameters is not usually practical, as a result correlations based on experimental measurements are used.

5.2. ECP Correlations

Due to the large number of parameters needed to fully characterize the ECP in the theoretical model, ECP correlations are developed from experimental data. Correlations for BWR coolant were developed by measuring ECP under simulated BWR coolant chemistry conditions using a rotating cylinder electrode (RCE) [Lin 1994]. The correlations used a hyperbolic tangent base model which includes terms to alter the slope to fit to the experimental data. The correlations developed take into account fluid velocity, hydrogen concentration, and either oxygen or hydrogen peroxide concentration. This results in two ECP values one for oxygen the other for hydrogen peroxide. The ECP correlation is given by the following equation and is valid for both oxidants:

$$ECP = C_1 \tanh\left[\frac{\log(Conc) - C_2}{C_3}\right] + C_4 \log(Conc) + C_5 \tag{5.4}$$

where: Conc: The oxidant concentration, O_2 or H_2O_2 in ppb
ECP: The ECP relative to the given oxidant in mV (SHE)

The five constants determine the shape of the curve with different constants used for oxygen and hydrogen peroxide. The constants for the hydrogen peroxide correlation are

$$C_1 = C_5 + 510 \tag{5.5}$$

$$C_2 = 0.00574\left[Conc_{H_2}\right]^{0.772} - 0.00754\sqrt{V_{RCE}} + 0.811 \tag{5.6}$$

$$C_3 = 0.569 \tag{5.7}$$

$$C_4 = 25.33 \tag{5.8}$$

$$C_5 = \frac{-4.62\left[Conc_{H_2}\right]^{0.808}}{e^{0.00280\left[Conc_{H_2}\right]}} + 1.50\sqrt{V_{RCE}} - 192.0 \tag{5.9}$$

The constants for the oxygen correlation are

$$C_1 = C_5 + 510 \tag{5.10}$$

$$C_2 = 0.00531\left[Conc_{H_2}\right]^{0.772} - 0.0111\sqrt{V_{RCE}} + 1.78 \tag{5.11}$$

$$C_3 = 1.02 \tag{5.12}$$

$$C_4 = 18.7 \tag{5.13}$$

$$C_5 = -18.6\left[Conc_{H_2}\right]^{0.264} - 177.0 \tag{5.14}$$

Where $Conc_{H2}$ is the hydrogen concentration in ppb and V_{RCE} is the velocity of the rotating cylinder electrode. The linear velocity in the BWR primary coolant path must be converted to this RCE velocity. The conversion is given by the following Equation:

$$V_{RCE} = 3.01e^{\left[0.425+1.25\ln\left(V_{pipe}\right)-0.179\ln\left(d_{pipe}\right)\right]} \tag{5.15}$$

Once the ECP is calculated for each oxidant the two must be combined to yield one ECP value for the region modeled. This is done using the following technique.

1. The two ECP values are calculated normally.
2. The values are compared with the largest value selected.
3. This value is used to determine an equivalent concentration of the other oxidant necessary to produce this ECP value. An example of this is given to clarify the technique. If the ECP due to hydrogen peroxide is found to

be the largest, the concentration of oxygen, i.e. equivalent concentration, needed to obtain this ECP value is calculated using the constants for the oxygen correlation, i.e. $Conc_{O_2} = f_{O_2}\left(ECP_{H_2O_2}\right)$. As the ECP correlation is not an easily invertable function the equivalent concentration is determined numerically using an iterative procedure.

4. The equivalent concentration is added to the original concentration which yielded the lower ECP value. Following the above example, the equivalent concentration is added to the oxygen concentration.

This new oxidant concentration is used in the correlation with the appropriate constants to calculate a final ECP for the region. Again with the above example the oxygen constants would be used.

The example described the actions if the hydrogen peroxide ECP was larger the process would be similar if the oxygen produced the higher ECP with the peroxide constants and concentrations being used instead of the oxygen.

5.2.1. Calculation of Rotating Cylinder Electrode Velocity

To compare the pipe and RCE velocities the mass transfer coefficients for the two are set equal to one another. The coefficient for the electrode is given by:

$$K_{RCE} = \left(\frac{f}{2}\right) V_{RCE} Sc_{RCE}^{-0.644} \tag{5.16}$$

where f is the friction factor given by:

$$\frac{f}{2} = \left(\frac{\tau}{\rho}\right) V_{RCE}^{-2} \tag{5.17}$$

the wall shear stress, τ, is given by:

$$\tau = 0.079\,\mathrm{Re}_{RCE}^{-0.3}\,\rho V_{RCE}^{2} \tag{5.18}$$

Substituting Eq. 5.17 and 5.18 into Eq. 5.16 gives the following equation in term of the Reynolds Number (Re), Schmidt Number (Sc), and RCE velocity.

$$K_{RCE} = 0.079\,\mathrm{Re}_{RCE}^{-0.3}\,V_{RCE}\,Sc_{RCE}^{-0.644} \tag{5.19}$$

Similarly the mass transfer coefficient for a pipe is given by:

$$K_{pipe} = 0.0889\frac{\sqrt{\tau}}{\rho}Sc_{pipe}^{-0.704} \tag{5.20}$$

The pipe wall shear stress is given by:

$$\tau = 0.04\,\mathrm{Re}_{pipe}^{-0.25}\,\rho V_{pipe}^{2} \tag{5.21}$$

Substituting Eq. 5.21 into 5.20 yields the following equation:

$$K_{pipe} = 0.0178\,\mathrm{Re}_{pipe}^{-0.125}\,V_{pipe}\,Sc_{pipe}^{-0.704}\,\rho^{-0.5} \tag{5.22}$$

Setting Eqs. 5.19 and 5.22 equal and substituting in the relationships for the Reynolds, $\nu V/d$, and Schmidt, ν/D, numbers yields the following equation for the RCE velocity:

$$V_{RCE}^{0.7} = 0.2253 V_{pipe}^{0.75}\frac{d_{RCE}^{0.3}}{d_{pipe}^{0.125}}\frac{D^{0.06}}{\nu^{0.235}\rho^{0.5}} \tag{5.23}$$

Using the RCE diameter of 2.5" and the water properties for 288°C water, ρ = 0.785 g/cm^3, ν = 1.29e-3 cm^2/sec, and $D^{0.06}$ = 0.64, gives the following simplified equation:

$$V_{RCE}^{0.7} = 1.35\frac{V_{pipe}^{0.75}}{d_{pipe}^{0.125}} \tag{5.24}$$

Eliminating the exponent of the RCE velocity term and converting the RCE velocity to rpm gives the following relationship used in the model.

$$V_{RCE} = 3.01e^{\left[0.425+1.25\ln\left(V_{pipe}\right)-0.179\ln\left(d_{pipe}\right)\right]} \quad (5.15)$$

Where V_{pipe} is in units of cm/sec and d_{pipe} is in units of cm.

6. Computer Simulation of BWR Water Chemistry

Boiling Water Reactors (BWRs) make up about 30% of the currently operating nuclear reactors worldwide [Chun 1990]. The current operational parameters are, a pressure of approximately 7.0MPa and a temperature of approximately 300°C. In the BWR steam is produced directly in the reactor vessel, in pressurized water reactors (PWRs) the steam is generated in a secondary loop isolating the steam turbines from radioactive materials. The disadvantage of this configuration, is that the steam produced in the reactor, contains radioactive gases requiring shielding of the turbine building.

The BWR reactor vessel, Figure 6.1, outer shell consists of the pressure vessel and the recirculation system. Inside the pressure vessel is the core shroud forming an annular region referred to as the downcomer. Inside the shroud are the core regions, consisting of the boiling and bypass regions, along with the upper plenum above them. The upper plenum is capped by the core shroud head dome on which are mounted the steam separator assemblies. The region around the steam separators is referred to as the mixing plenum. The final region, beneath the core, is called the lower plenum.

6.1. Description of BWR Primary Coolant Path

The flow path of the primary coolant through the BWR vessel and the recirculation system is as follows beginning with the feedwater inlet:

1. The steam that passed through the turbines and other secondary system components enters the vessel as feedwater.

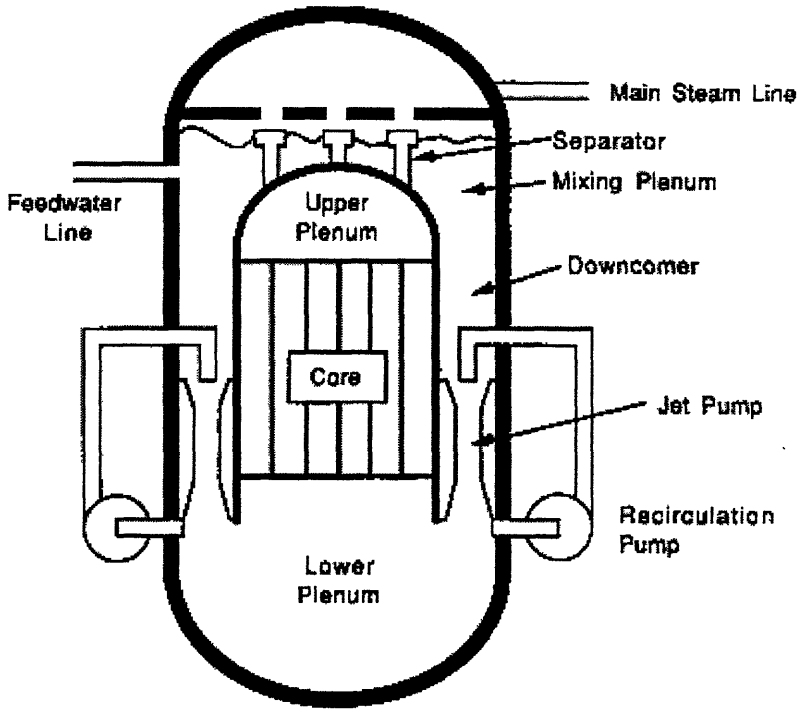

Figure 6.1 BWR Reactor Vessel Schematic

2. The feedwater enters the mixing plenum where it mixes with the saturated liquid from the moisture separator.

3. The combined coolant then enters the downcomer region.

4. The coolant passes through the jet pump into the lower plenum with a fraction of the flow diverted into the recirculation line to power the jet pump.

5. The coolant enters the lower plenum and is transported into the core.

6. Most of the coolant enters the boiling region and is converted to a two-phase mixture. The remainder of the coolant remains liquid and passes through the bypass region.

7. The flow from the two regions recombine in the upper plenum and is transported through to the moisture separator.

8. The saturated vapor is separated and is transported via the main steam lines to the turbines and condensers back to the feedwater inlet. The

saturated vapor is separated and is transported directly to the mixing plenum. The cycle then repeats.

6.2. Modeling of BWR Regions

To model chemical concentrations and electrochemical corrosion potential along the BWR flow path, thermal-hydraulic and radiation dose profiles are used. To do this accurately any region along the BWR primary coolant loop where these parameters change substantially must be individually modeled. These individual regions are referred to as components in the RADICAL model. The current BWR model uses 30 components joined at 18 nodes as shown in **Figure 6-2**.

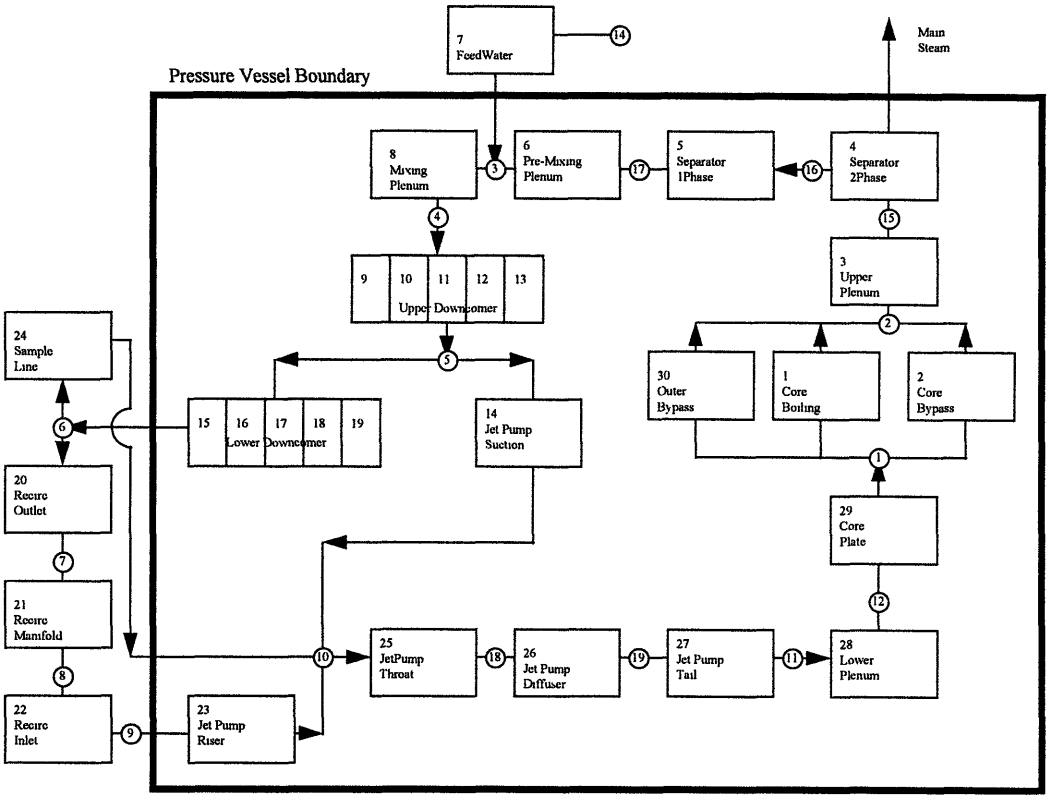

Figure 6-2 BWR Component Schematic

The various components are described in subsequent sections and are shown in relation to each other in **Figure 6-3**.

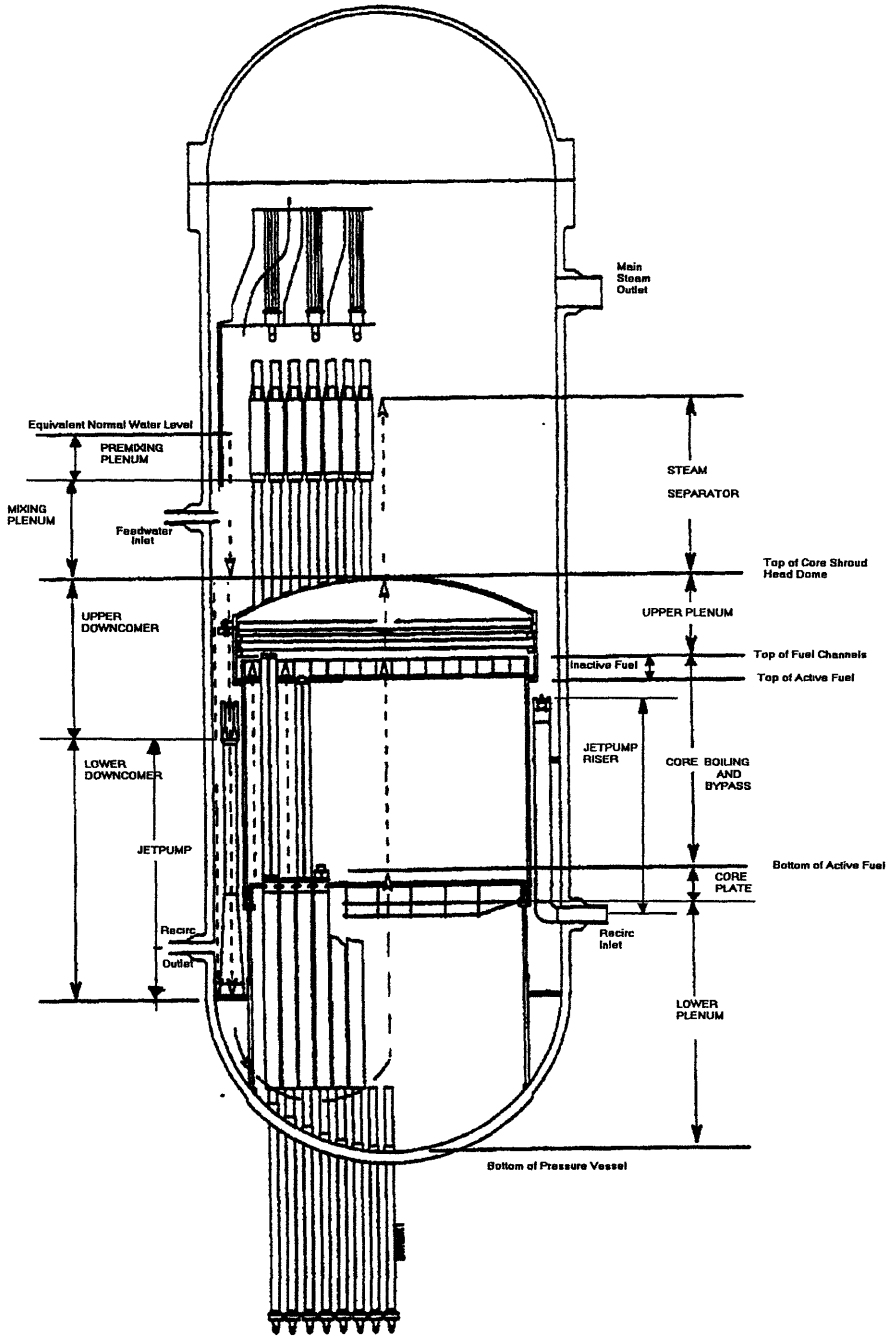

Figure 6-3 Location of Components within the BWR Pressure Vessel

6.2.1. Core

The core is modeled as three parallel flow components core boiling, core bypass, and outer bypass. The core boiling component consists of the fraction of core flow which passes through the fuel bundles. The flow through this component is two-phase. The core bypass component is the fraction of flow through the core which passes between the fuel bundles. The flow in this component remains single-phase. The outer bypass component consists of the fraction of flow between the periphery of the fuel bundles and the core shroud. The flow in this component also remains single-phase. The three core components are parallel components with identical vertical dimensions.

6.2.2. Upper Plenum

The upper plenum component represents the region inside the core from the top of the active fuel to the top of the core shroud head dome. The concentrations in this area are calculated based on a mass flow averaged value of the concentrations from the core boiling, core bypass, and outer bypass components.

6.2.3. Steam Separator

The steam separator region is schematically illustrated in Figure 6.4 and is modeled as two components, a two-phase and a single-phase component. The two-phase component consists of the standpipes above the core shroud head dome and the central core of the steam separator assembly. The single-phase

component represents the annular flow around the outside of the steam separator central core.

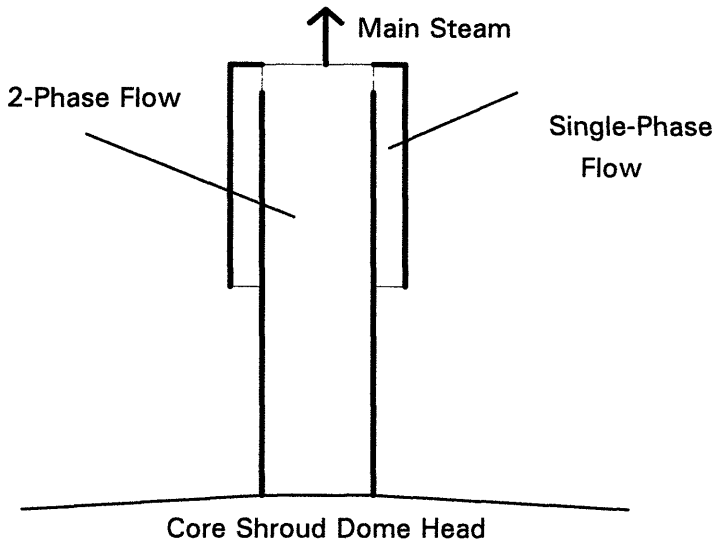

Figure 6-4. Steam Separator Component Schematic

6.2.4. Mixing Plenum

The mixing plenum is the region of the reactor above the core shroud head dome surrounding the steam separator assemblies. This region is also split into two components, premixing and mixing. The premixing component is the region from the bottom of the steam separator assemblies to the top of the pressure vessel liquid level. The flow in this component consists only of the flow exiting from the single-phase steam separator component.

The mixing component is the region between the bottom of the separator to the top of the core shroud head. The flow in this component consists of both the flow exiting the single-phase steam separator component but also the flow added to simulate the addition of feedwater.

6.2.5. Downcomer

The downcomer is divided into two axial super-components, the upper downcomer and the lower downcomer. The upper downcomer component consists of the region between the top of the core shroud head dome and the suction inlet of the jet pumps. The lower downcomer consists of the area from the jet pump suction inlet to the bottom of the downcomer channel not including the jet pump assemblies. The flow through the upper downcomer consists of the total mass flow rate of the primary system. The flow through the lower downcomer consists of the fraction of flow which enters the recirculation system. To better represent the doserates inside the downcomer the two axial super-components are arbitrarily divided into five, any number of divisions is possible, equal radial width components schematically illustrated in **Figure 6-5**. The fraction of flow through each is set to the fraction of total cross-sectional area calculated for that component. In the upper downcomer this is simply the ratio of the component annular area to the super-component annular area. In the lower downcomer these areas need to be adjusted to subtract the area of the jet pump assemblies from the area of the components through which they pass. The dose rates at the center of each section are adjusted assuming exponential attenuation of the radiation.

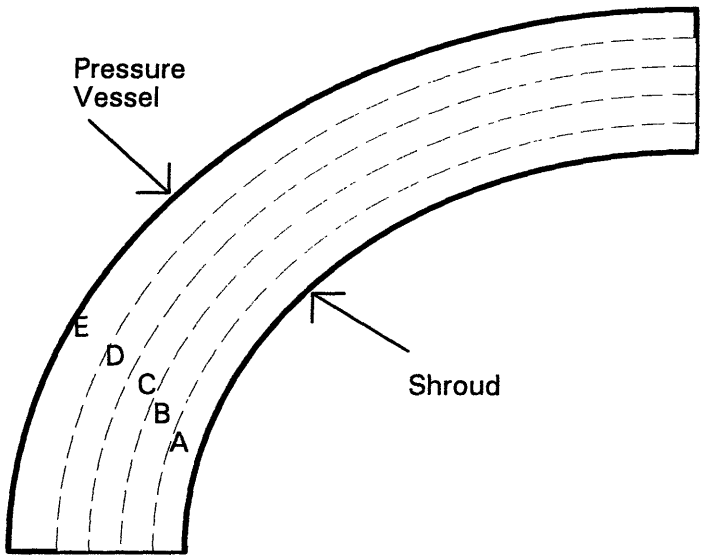

Figure 6-5 Downcomer Radial Sections

6.2.6. Recirculation Line

The recirculation line is divided into four axial components recirc outlet, recirc manifold, recirc inlet, and jet pump riser. The recirc outlet component is the region of the recirculation lines from the pressure vessel penetration at the bottom of the lower downcomer to the entrance of the manifold. The recirc manifold component is the region of the recirculation lines between the outlet pipes and the inlet pipes which carry flow to the jet pumps. The recirc inlet component is the region between the manifold and the 90 degree bend in the recirculation piping located in the downcomer region. The jet pump riser component is the final region consisting of the portion of the recirculation line which is vertically aligned inside the downcomer between the two jet pumps it supplies driving flow to. The jet pump riser is the only component exposed to a radiation field.

6.2.7. Jet Pump

The jet pump region is divided into three components, the throat, diffuser, and tail. The jet pump throat component is the region from the inlet suction opening in the downcomer to where the cross-sectional area begins to expand. The jet pump diffuser component is the region where the cross-sectional area increasing along its axial length. The jet pump tail component is the region at the end of the diffuser with a constant axial cross-sectional area ending at the bottom of the downcomer. These regions are schematically illustrated in **Figure 6-6**.

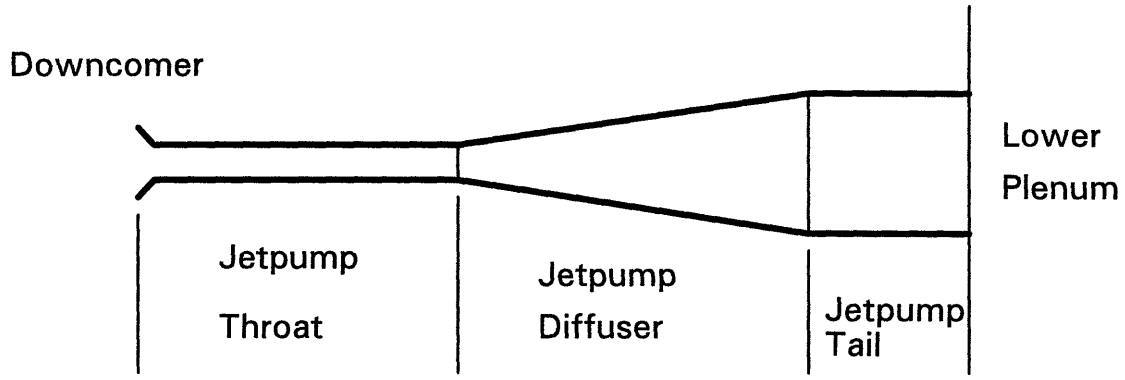

Figure 6-6 Jet pump Model Schematic

6.2.8. Lower Plenum

The Lower Plenum is divided into two axial components, lower plenum and core plate. The lower plenum component consists of the region forming the bottom of the pressure vessel below the downcomer and the core plate. The core plate component represents the region beginning at the bottom of the core plate structure and ends at the bottom of the active fuel. This component separate as it is the region exposed to the radiation field.

6.2.9. Sample Line

The sample line is a component which has been added to simulate the effects of water sampling in order to compare RADICAL results to plant measurements. This component is modeled as a 1/4 inch diameter pipe 20 meters long. The fraction of flow through this component is one-millionth of the total flow. This flow is artificially reintroduced into the loop at the jet pump in order to maintain conservation of mass in the loop. While chemical reactions alter the concentrations in this component, the small flow rate results in a minor, approximately 0.001 ppb or less, difference in the concentration at the jet pump.

7. RESULTS

The purpose of the RADICAL code is to implement the model for water chemistry and ECP for a BWR primary coolant system as accurately as possible, while keeping the operational time short enough to provide 'real-time' modeling. In order to better model the chemistry and ECP the model was modified to allow characterization of variable cross-sectional area flow regions. To test the accuracy of the model simulations were conducted for a typical BWR-3 and BWR-4 with the results compared with actual plant data for hydrogen and oxygen concentrations measured in the recirculation line. Parametric studies were conducted for the BWR-3 to determine the effect of various physical parameters on the calculated species concentrations to focus further development of input file parameter accuracy. In addition to these parametric studies, additional simulations were run to evaluate the effect of varying the power and flow within the allowable operating ranges for a BWR on both species concentrations and ECP.

Most parameters used to model the BWR-3 and BWR-4 were obtained from a proprietary EPRI report [Romeo 1995] and as a result cannot be published in this thesis. In addition the dimensions used for modeling the jet pump, steam separator, and recirculation line hydraulic diameters and cross-sectional flow areas were taken from the FSAR for the Pilgrim Power Plant [1970] and were considered to be typical for both plants studied.

7.1. Variable Area Modeling

As mentioned previously one major modification to the model was to allow for the use of variable cross-sectional area components. The current BWR model only uses this ability in modeling the Jet Pump Diffuser component. To determine the effect this modification had on the model, two simulations were run with the only difference in the diffuser region. The first simulation set the average area of the diffuser to be constant along its axial length. The second simulation was done modeling the area as a linear interpolation between the entrance and exit cross-sectional areas.

A comparison of oxygen and hydrogen peroxide concentrations for the jet pump is displayed in Figure 7.1 for a hydrogen injection level of 1 ppm, hydrogen was excluded as it showed little variability through the jet pump.

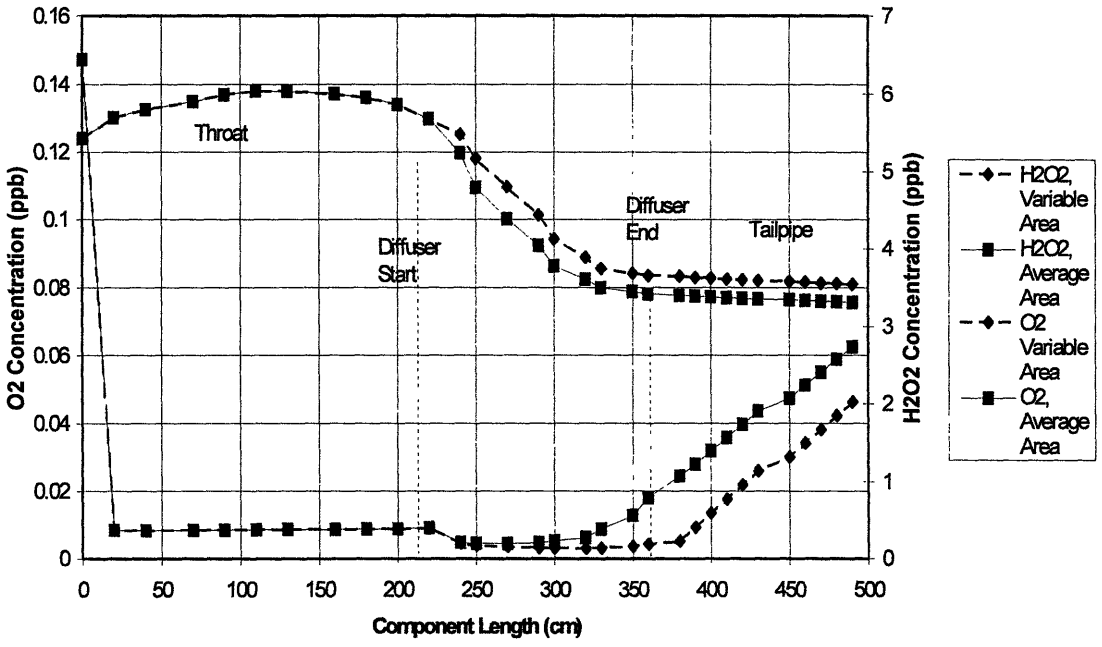

Figure 7.1 Comparison of Species Concentrations for the Jet Pump Models

Figure 7.1 shows a definite change in species concentration at the beginning of the diffuser region. This difference is primarily due to the high initial velocity allowing little time for peroxide decomposition at the beginning of the diffuser. Once the flow has slowed farther down the jet pump the surface decomposition of peroxide is impeded due to the larger hydraulic diameter than in the average area model. As a result more peroxide, and correspondingly less oxygen remains at the exit of the jet pump diffuser. The resulting exit concentrations then effect the tailpipe concentrations.

Figure 7.2 shows the ECP for the same two simulation runs. The average area shows dramatic jumps at the beginning and end of the diffuser due to the discontinuity in water velocity.

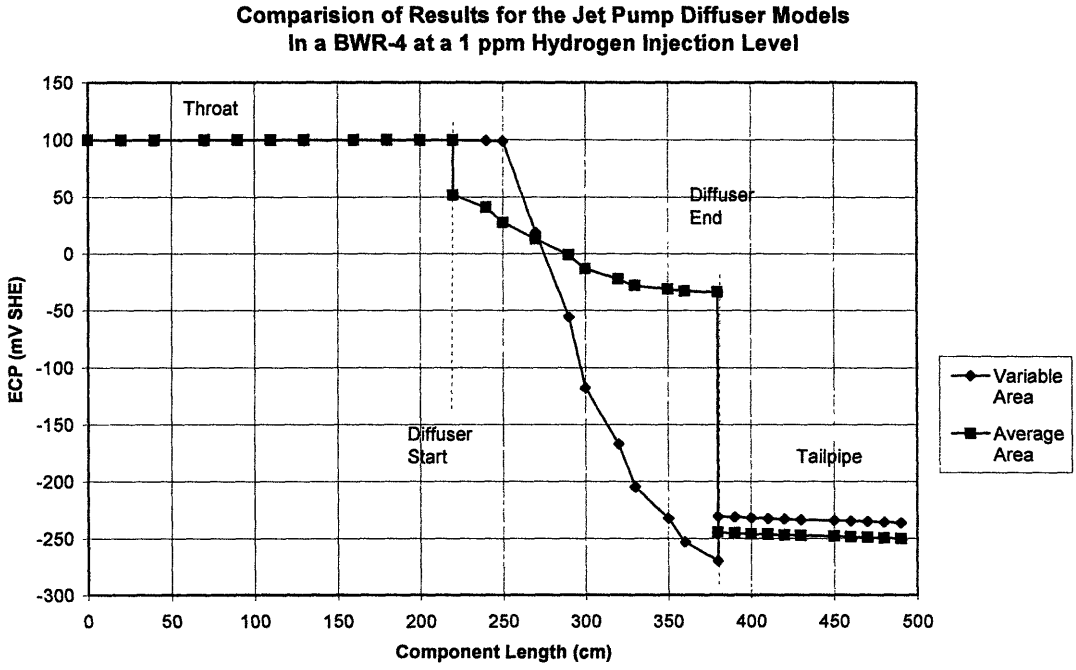

Figure 7.2 Comparison of ECP for the Jet Pump Models

This is not present with the variable area model where the ECP initially continues at the same value as the throat due to the higher concentrations of peroxide as well as the high velocity. A smooth transition along the diffuser length follows with a small jump at the tailpipe possibly due to a cessation of radiation dose at this point. As these Figures show variable area modeling can not only have significant impact on the loop concentrations, it also is important within components to show the variability along the axial length.

7.2. Normal Water Chemistry

Normal water chemistry is the term used for the operating condition where no hydrogen is injected in the feedwater system. Simulations were run for this condition for both a typical BWR-3 and BWR-4. The results of these simulations are shown in Figures 7.3 through 7.16 for the BWR-3 and Figures 7.17 through 7.30 for the BWR-4. The primary coolant flow path has been divided into seven sections for viewing convenience. Each of the seven sections has two figures associated with it. The first is a plot of the hydrogen, oxygen, and hydrogen peroxide concentrations along the flow path. The second is the electrochemical corrosion potential resulting from these concentrations and the flow velocity.
In the core section, Figures 7.3 and 7.17, radiolysis dominates at first rapidly building the concentrations of hydrogen and hydrogen peroxide, oxygen is not a direct product of radiolysis. Once the concentrations build to a high enough value chemical reactions occur rapidly enough to establish an equilibrium concentration over most of the bypass region, this is the case for the entire outer

bypass region which does not have as high a doserate compared to the inner core. At the end of the core region recombination begins to dominate as the dose drops lowering all the concentrations. The other noticeable effect is at the onset of boiling the hydrogen levels drop rapidly due to stripping of the hydrogen into the vapor phase. This stripping also boosts the oxygen concentration as there is less hydrogen available for recombination despite stripping of oxygen also. Examining the ECP for the two reactors, Figures 7.4 and 7.18, the core bypass has the lowest ECP due to the high production of hydrogen along with the absence of hydrogen stripping which raises the relative ECP of the core boiling. The outer bypass has the highest ECP as a result of little hydrogen production by radiolysis as would be expected from mixed potential theory.
In the upper plenum and steam separator section, Figures 7.5 and 7.19, The concentrations from the three core regions combine and stabilize at first to the new thermal hydraulic and radiation levels. At this point hydrogen peroxide decomposition dominates the chemical reactions forming primarily oxygen, hence the mirror image profile of these lines. The upper plenum having a large hydraulic diameter effects peroxide minimally however when entering the steam separators the hydraulic diameter shrinks rapidly causing the rapid decrease in peroxide concentration. The ECP in this section, Figures 7.6 and 7.20, again stabilizes to the parameters and remains constant across the upper plenum at the steam separators there is a rapid area reduction, velocity increase, resulting in the dramatic jump in ECP. A second smaller jump is seen at the transition between 2-phase and 1-phase flow where there is a slight velocity drop.

The mixing plenum, Figures 7.7 and 7.21, show the same initial stabilization and peroxide decomposition traits. The discontinuity at the midpoint of the section represents the point at which feedwater is introduced to the primary coolant adjusting the concentrations appropriately. The same behavior is seen in the ECP, Figure 7.8 and 7.22.

The downcomer section, Figures 7.9 and 7.23, is a mass averaged combination of the five radial model components. In this region radiation levels begin to climb, primarily gamma, with the produced species stimulating recombination of hydrogen and oxygen as peroxide builds up slightly. After the first third of the downcomer a majority of the flow enters the jet pump reducing the flow velocity in the remainder of the region, where further recombination occurs to an equilibrium point. In the lower downcomer surface decomposition of peroxide is enhanced by the additional surfaces of the jet pump assemblies. The ECP for this section, Figures 7.10 and 7.24, increases due to the recombination of hydrogen, drops as the velocity drops, and climbs again as recombination continues.

In the recirculation line, Figures 7.11 and 7.25, decomposition of peroxide on the pipe walls dominate the reactions up to the final portion, the jet pump riser, where radiation levels are similar to those inside the downcomer resulting in recombination and peroxide production. The ECP, Figures 7.12 and 7.26 remain steady except where pipe diameters shift, hence velocity changes, and at the end where the recombination of hydrogen increases the ECP.

In the jet pump, Figures 7.13 and 7.27, the velocity is so high that there is insufficient time for any major changes to occur in species concentrations. However the ECP, Figures 7.14 and 7.28, varies as the cross-sectional area effects the velocity.

In the lower plenum, Figure 7.15 and 7.29, peroxide decomposition is the dominant effect until the end of the section as the fluid reenters the core's radiation field rapidly building up all species. The ECP, Figures 7.16 and 7.30, remains steady until the production buildup where the rapid increase in hydrogen drops the ECP.

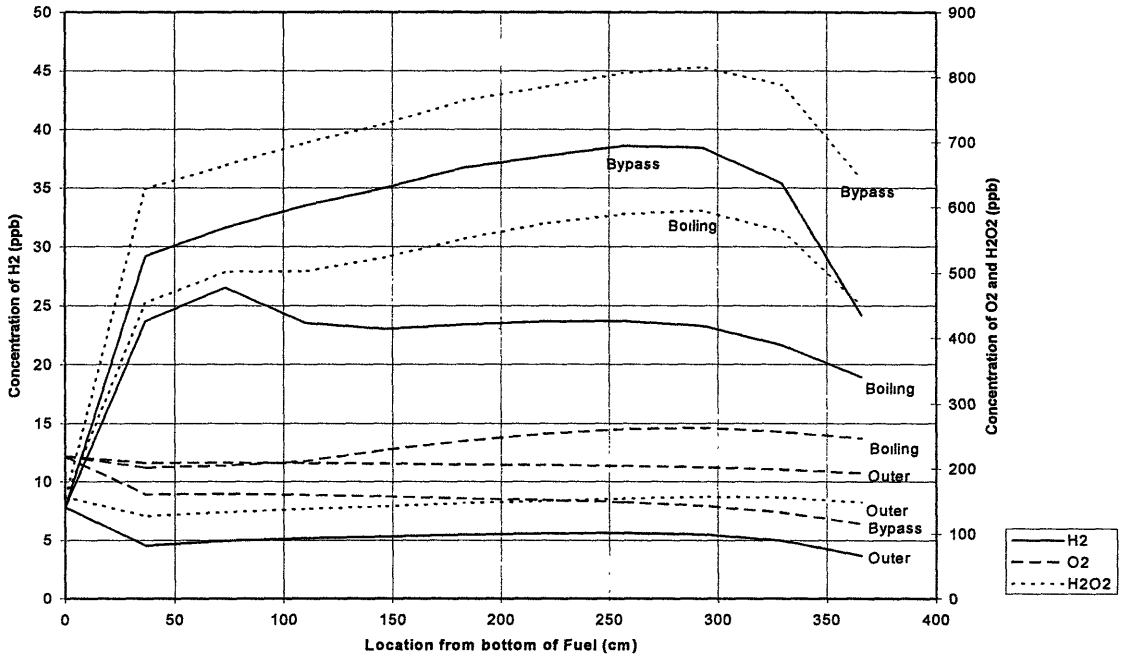

Figure 7.3 BWR-3 Core Species Concentrations

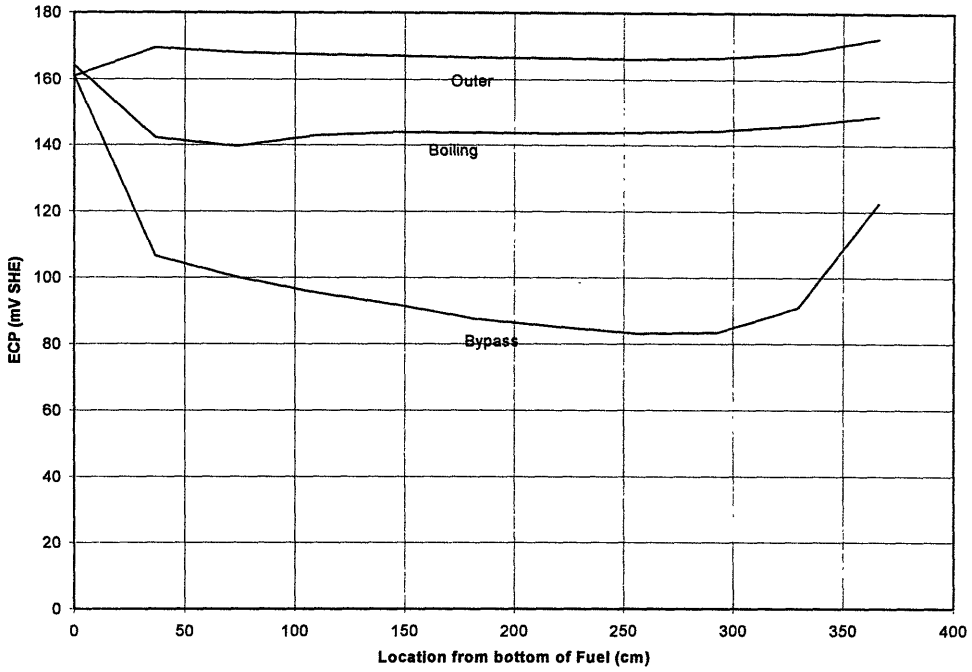

Figure 7.4 BWR-3 Core ECP

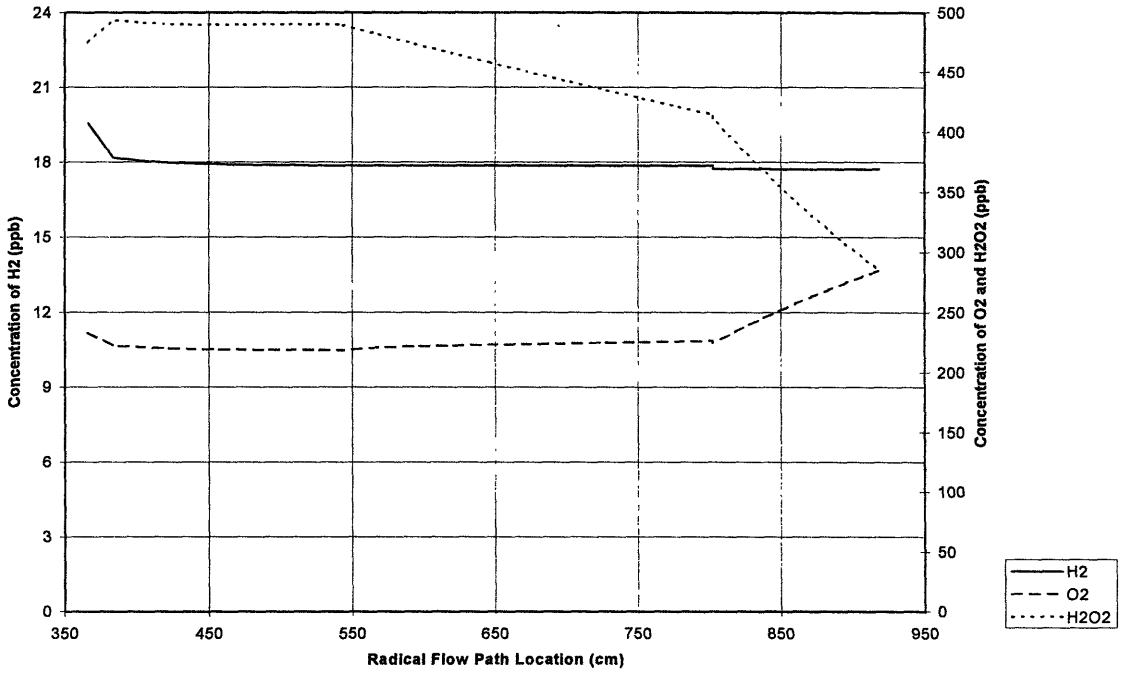

Figure 7.5 BWR-3 Upper Plenum and Steam Separator Species Concentrations

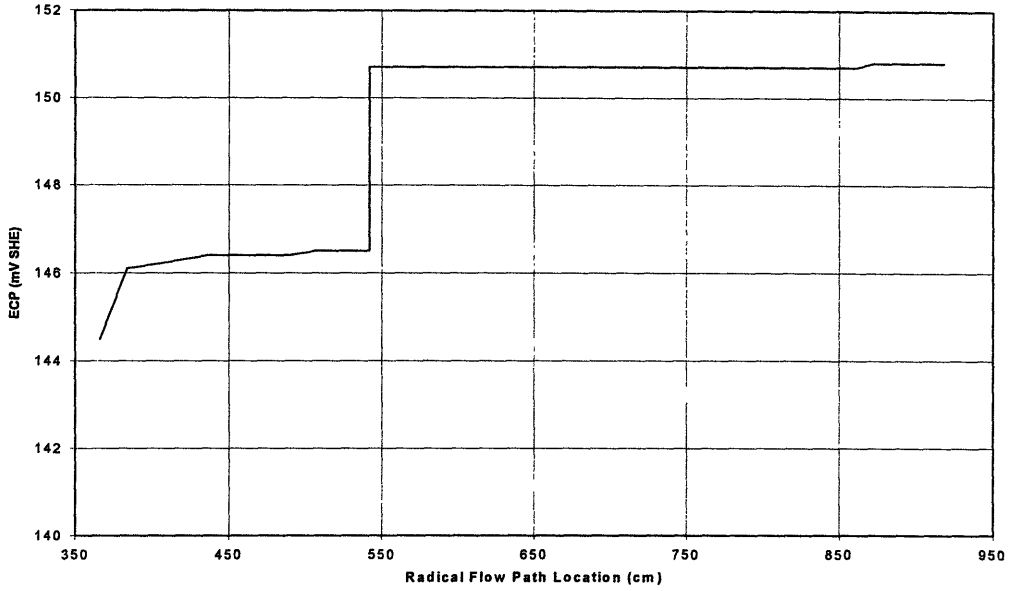

Figure 7.6 BWR-3 Upper Plenum and Steam Separator ECP

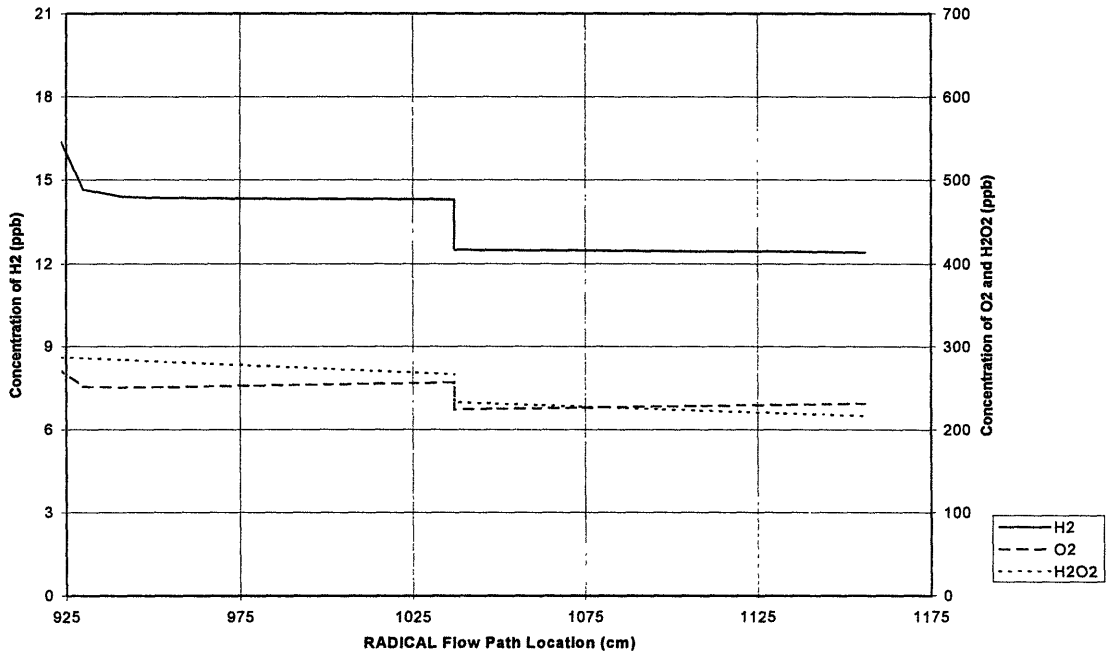

Figure 7.7 BWR-3 Mixing Plenum Species Concentrations

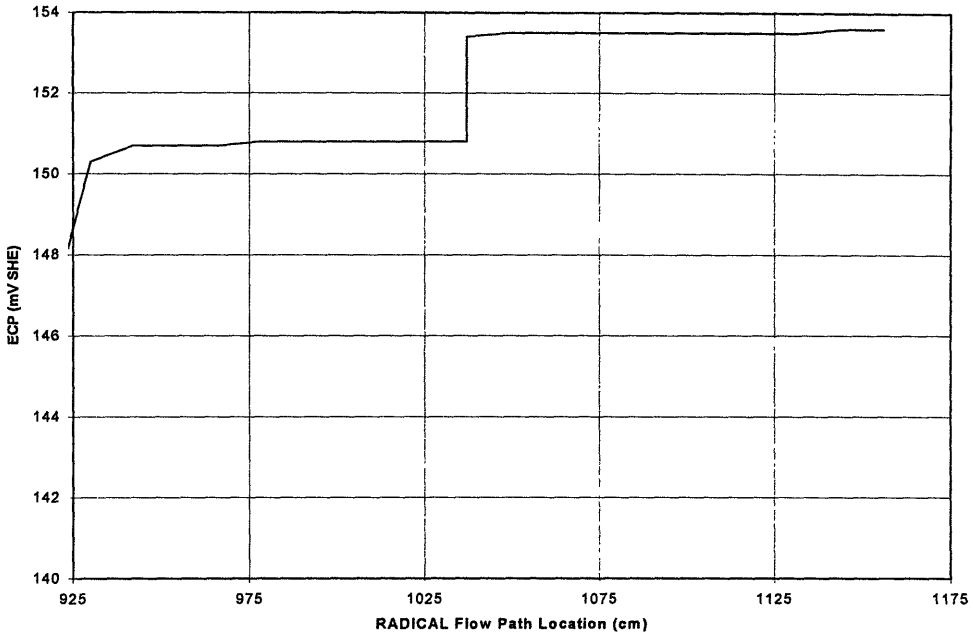

Figure 7.8 BWR-3 Mixing Plenum ECP

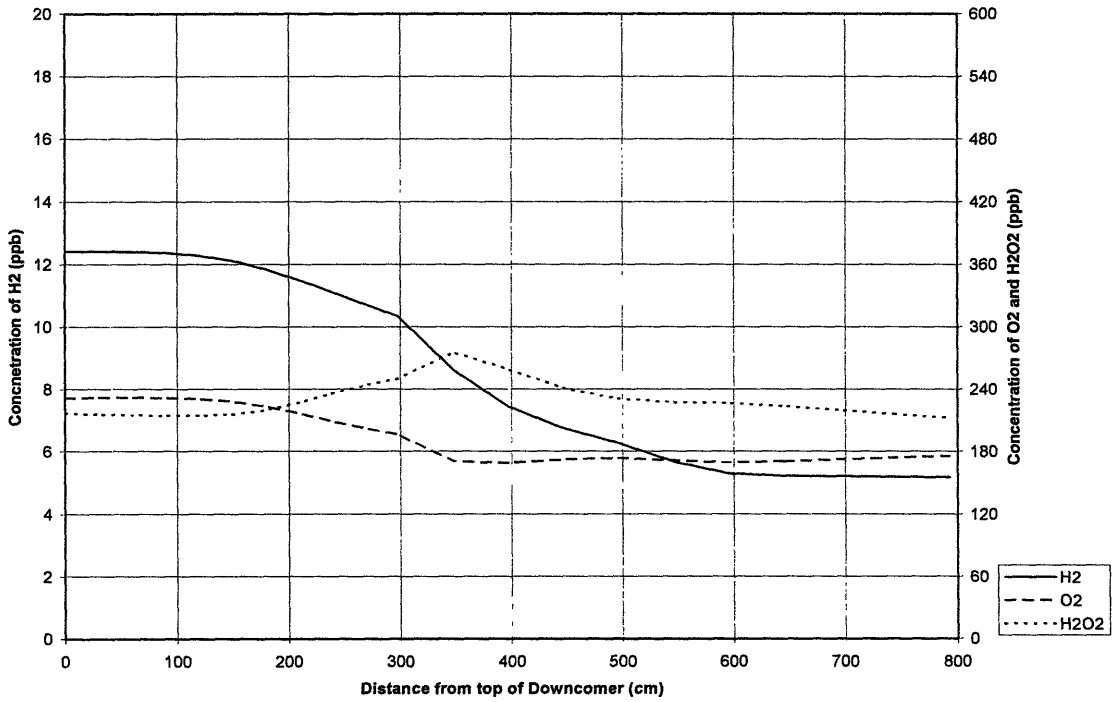

Figure 7.9 BWR-3 Downcomer Species Concentrations

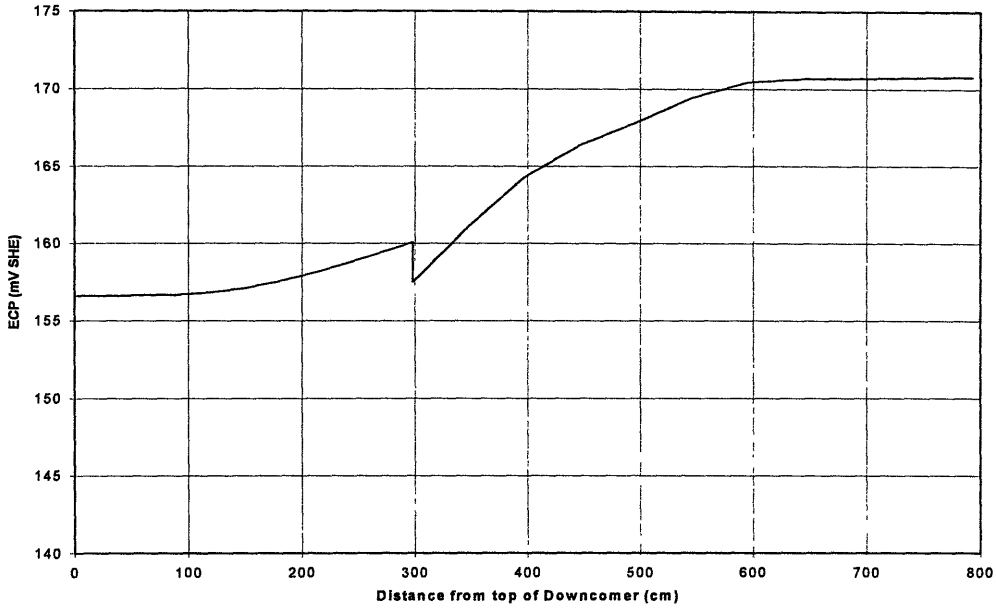

Figure 7.10 BWR-3 Downcomer ECP

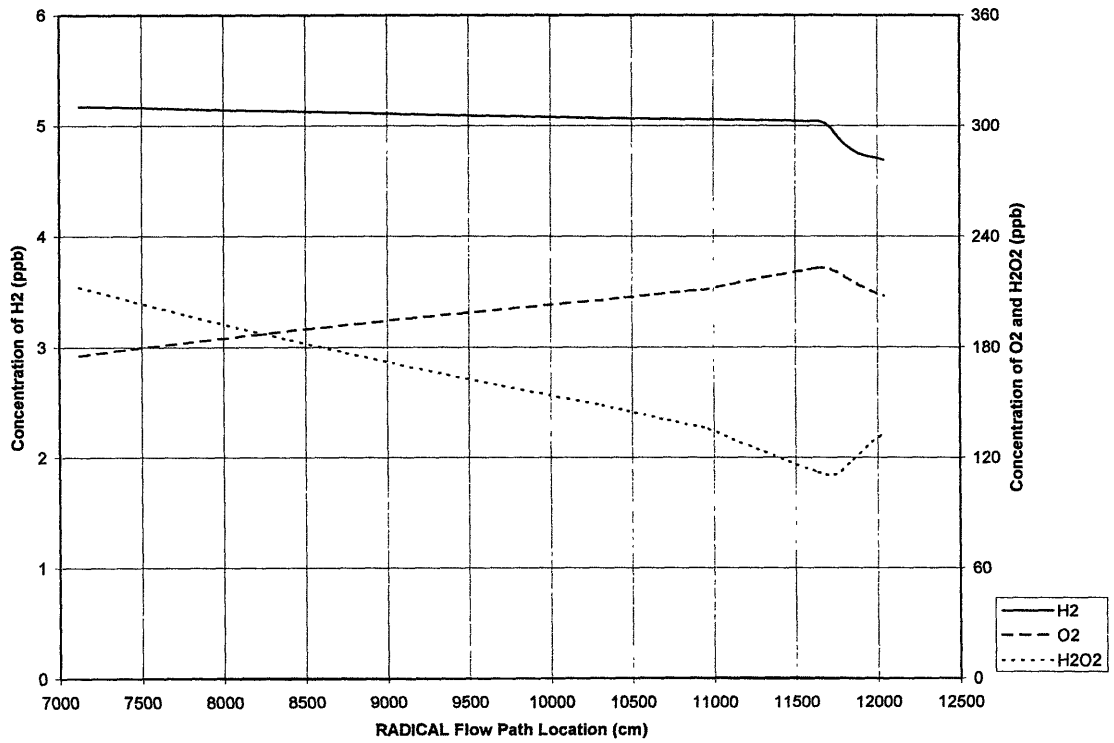

Figure 7.11 BWR-3 Recirculation Line Species Concentrations

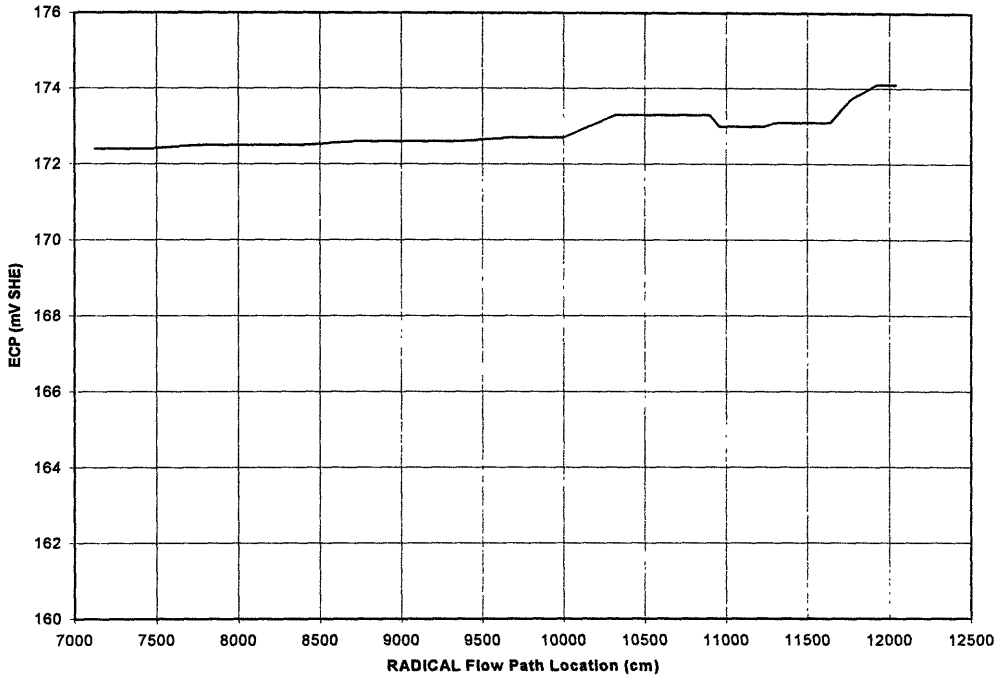

Figure 7.12 BWR-3 Recirculation Line ECP

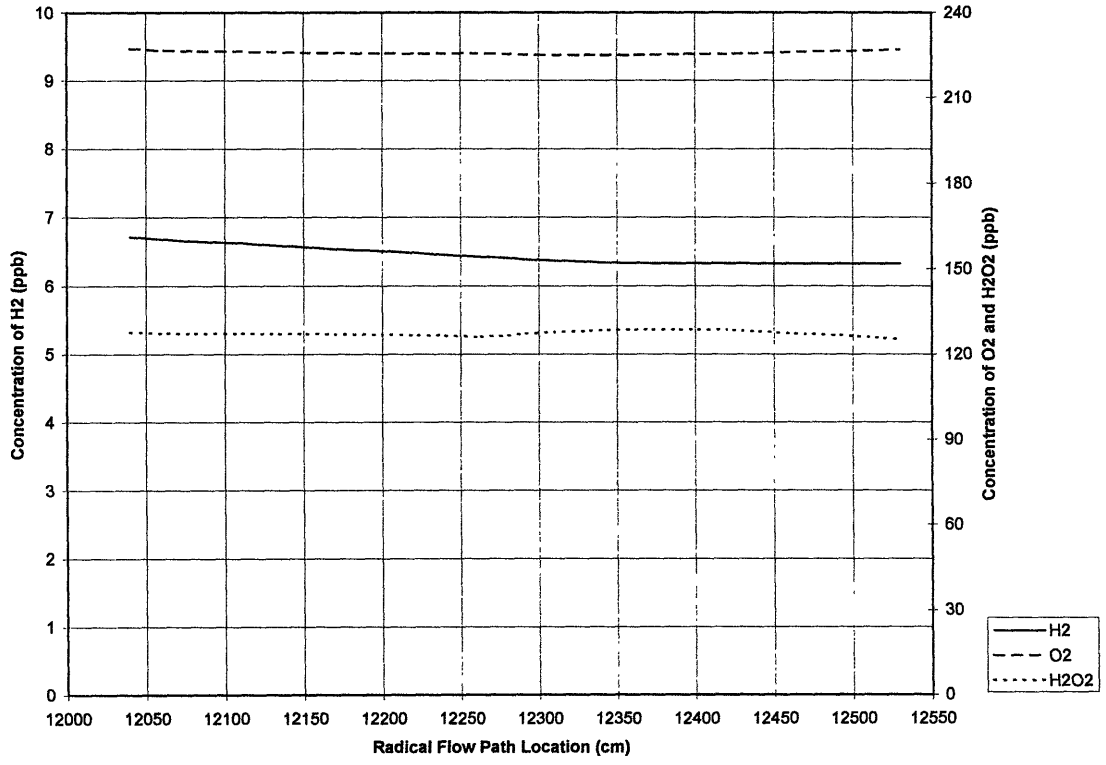

Figure 7.13 BWR-3 Jet Pump Species Concentrations

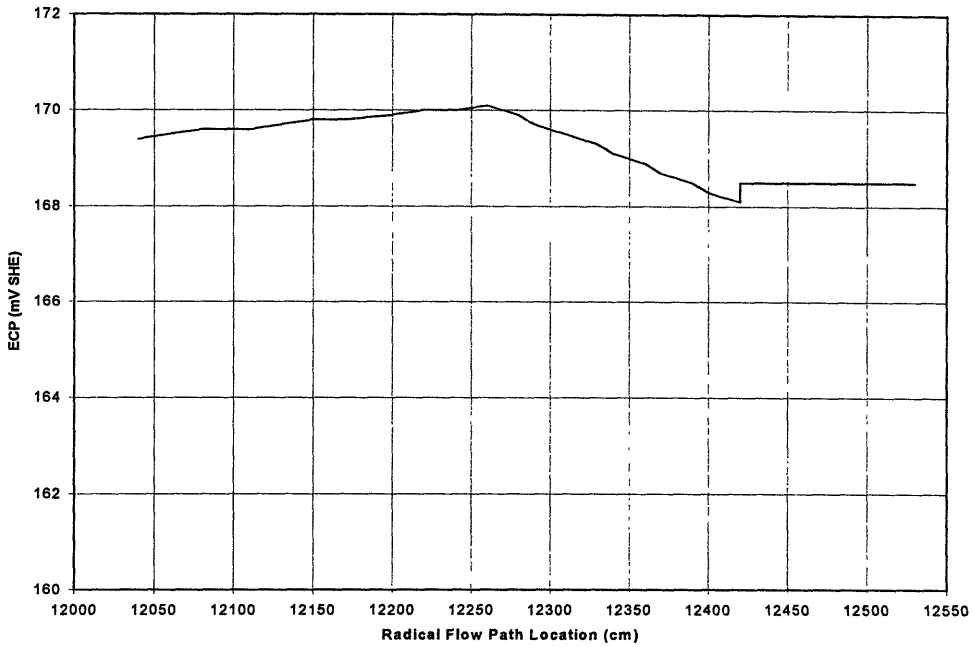

Figure 7.14 BWR-3 Jet Pump ECP

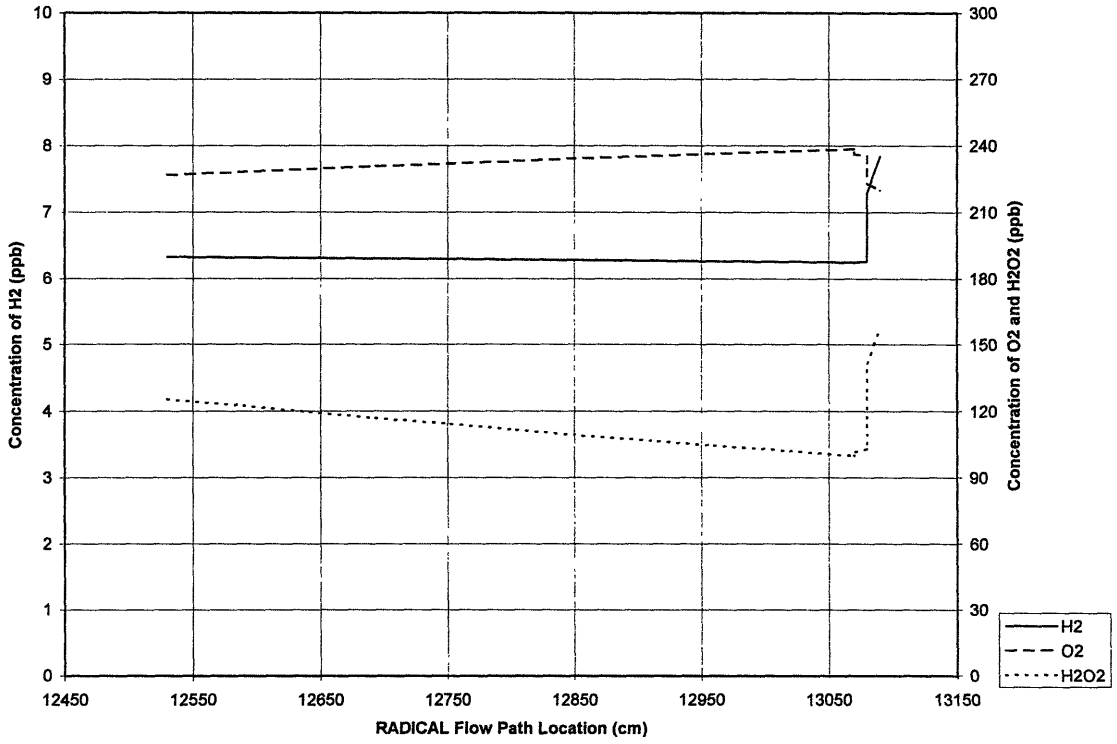

Figure 7.15 BWR-3 Lower Plenum Species Concentrations

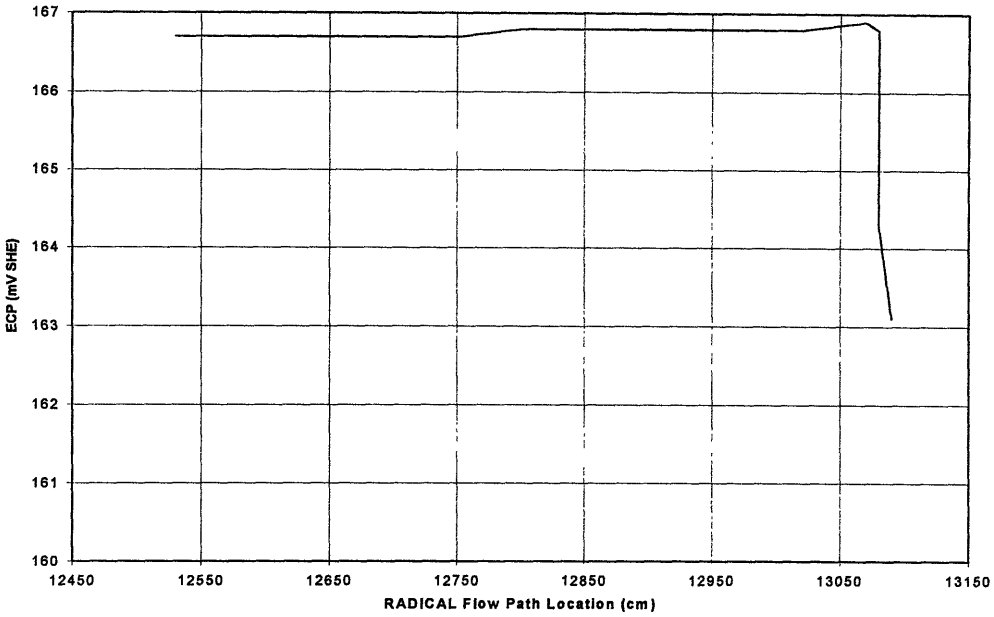

Figure 7.16 BWR-3 Lower Plenum ECP

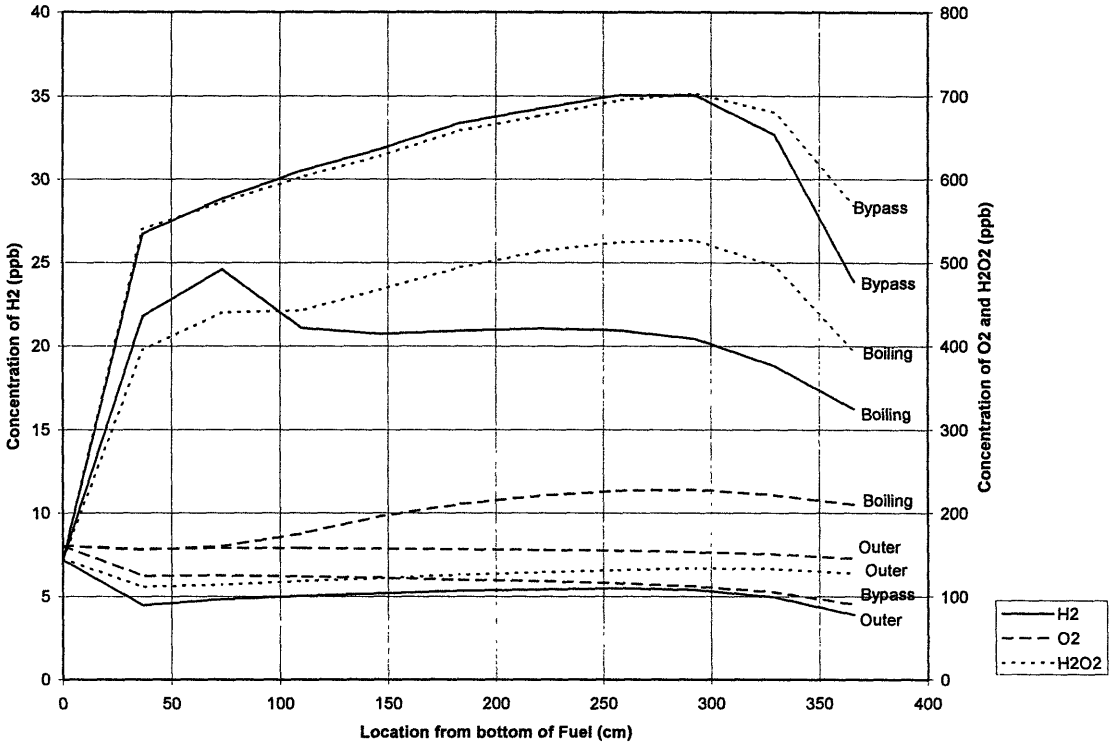

Figure 7.17 BWR-4 Core Species Concentrations

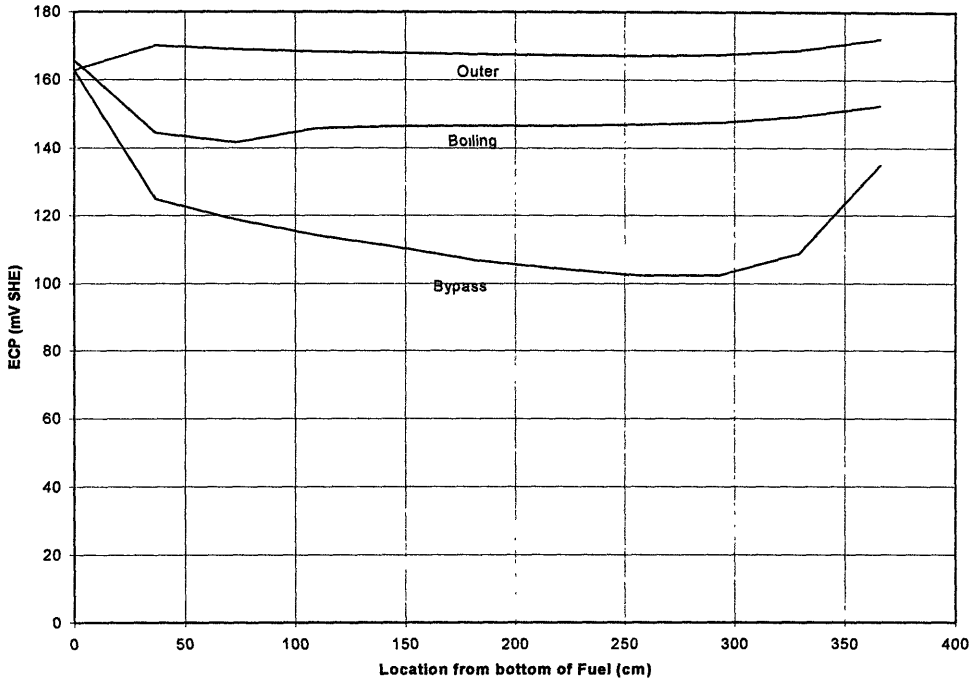

Figure 7.18 BWR-4 Core ECP

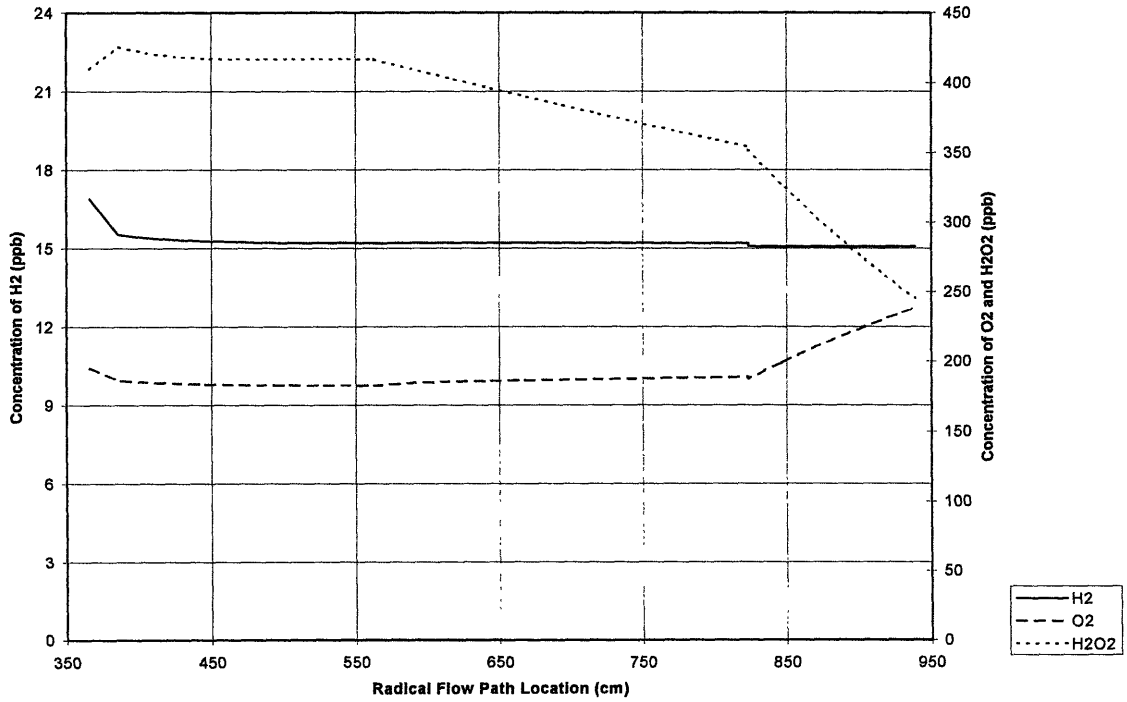

Figure 7.19 BWR-4 Upper Plenum and Steam Separator Species Concentrations

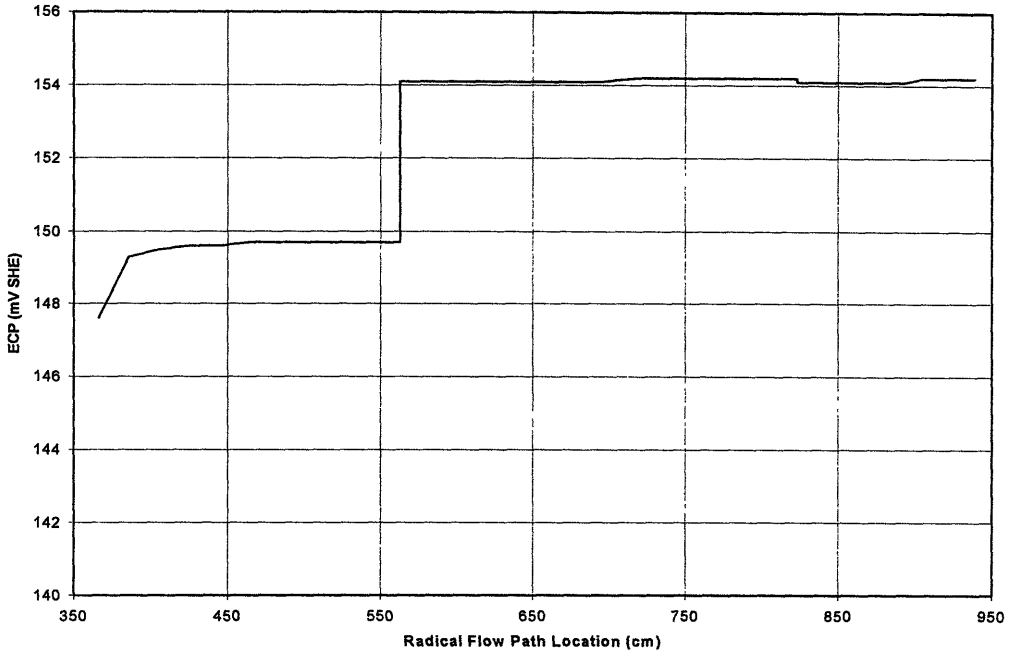

Figure 7.20 BWR-4 Upper Plenum and Steam Separator ECP

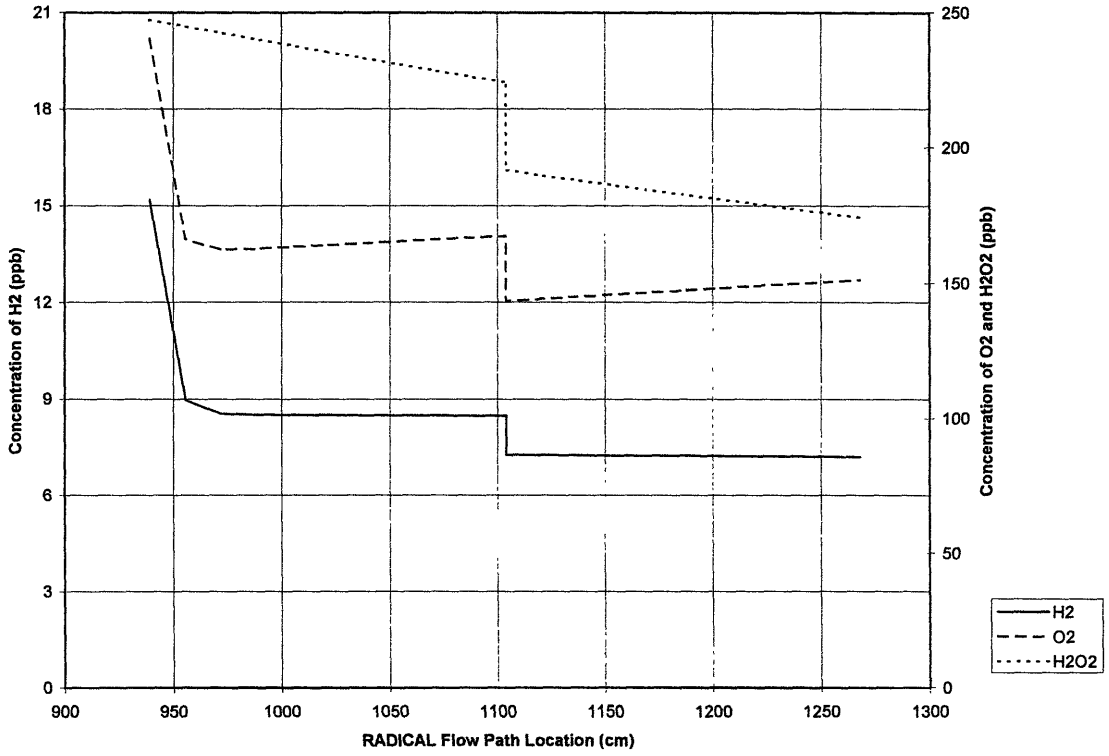

Figure 7.21 BWR-4 Mixing Plenum Species Concentrations

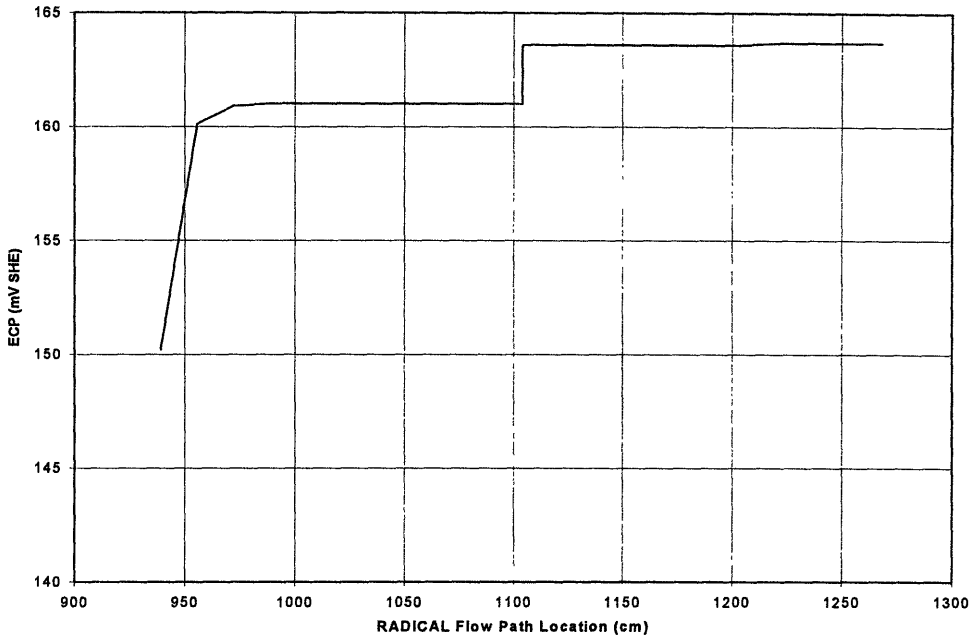

Figure 7.22 BWR-4 Mixing Plenum ECP

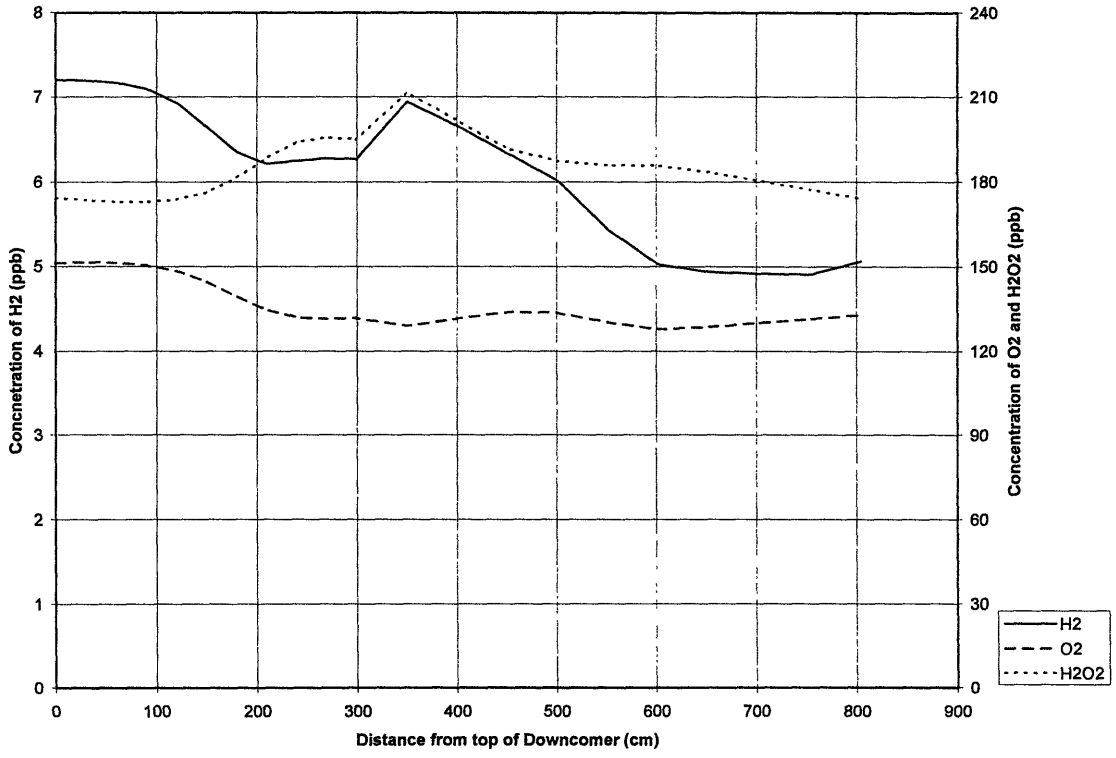

Figure 7.23 BWR-4 Downcomer Species Concentrations

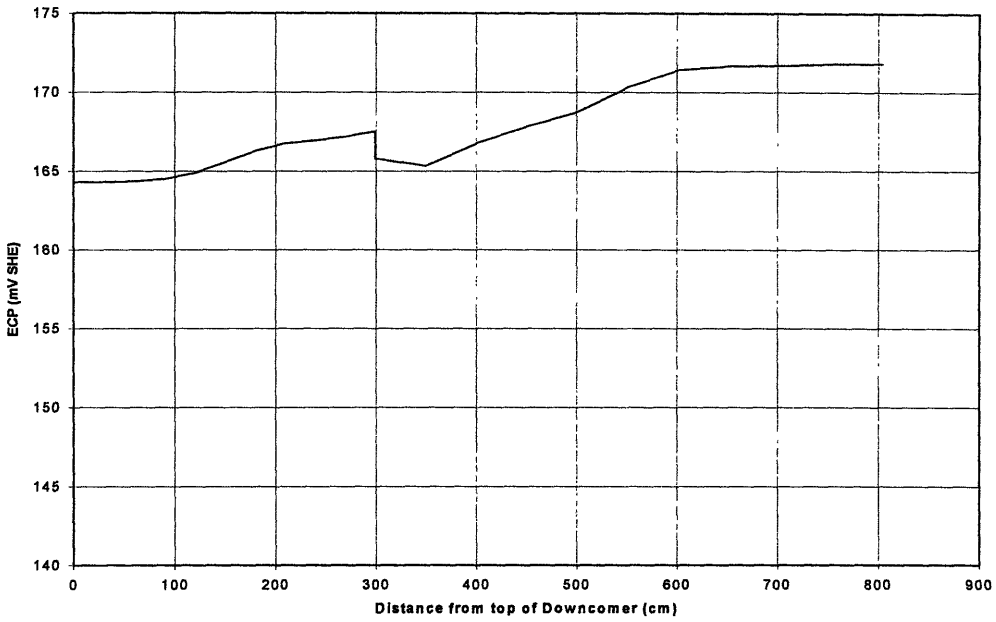

Figure 7.24 BWR-4 Downcomer ECP

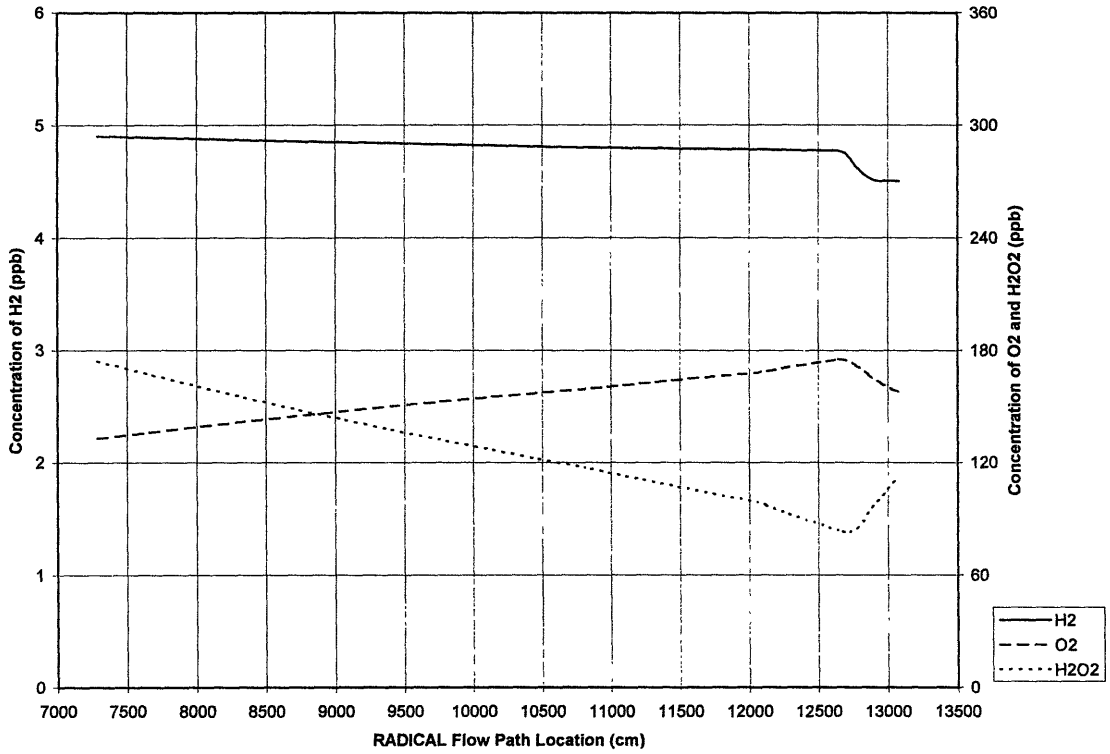

Figure 7.25 BWR-4 Recirculation Line Species Concentrations

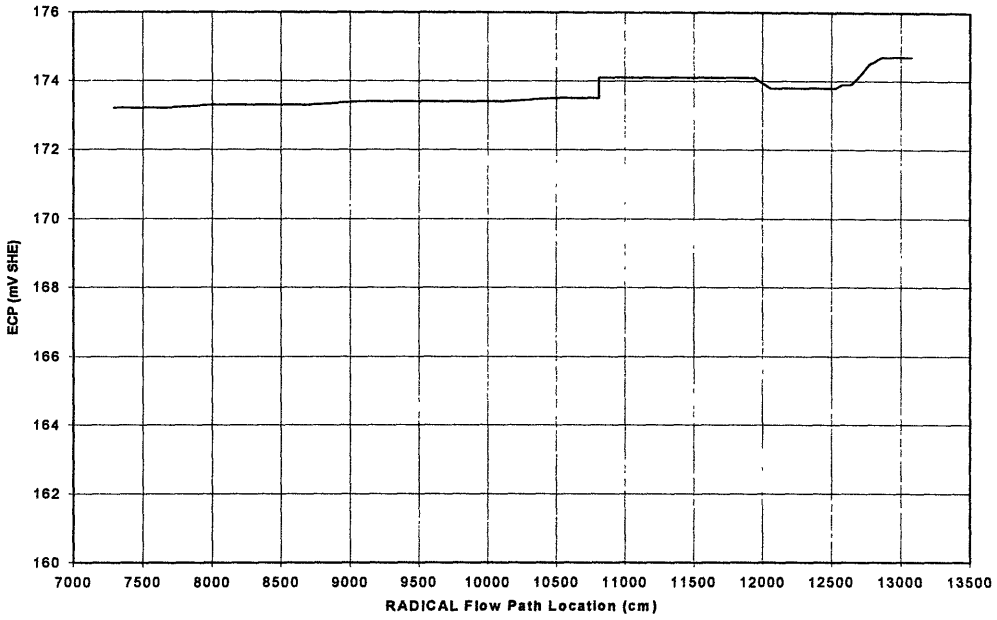

Figure 7.26 BWR-4 Recirculation Line ECP

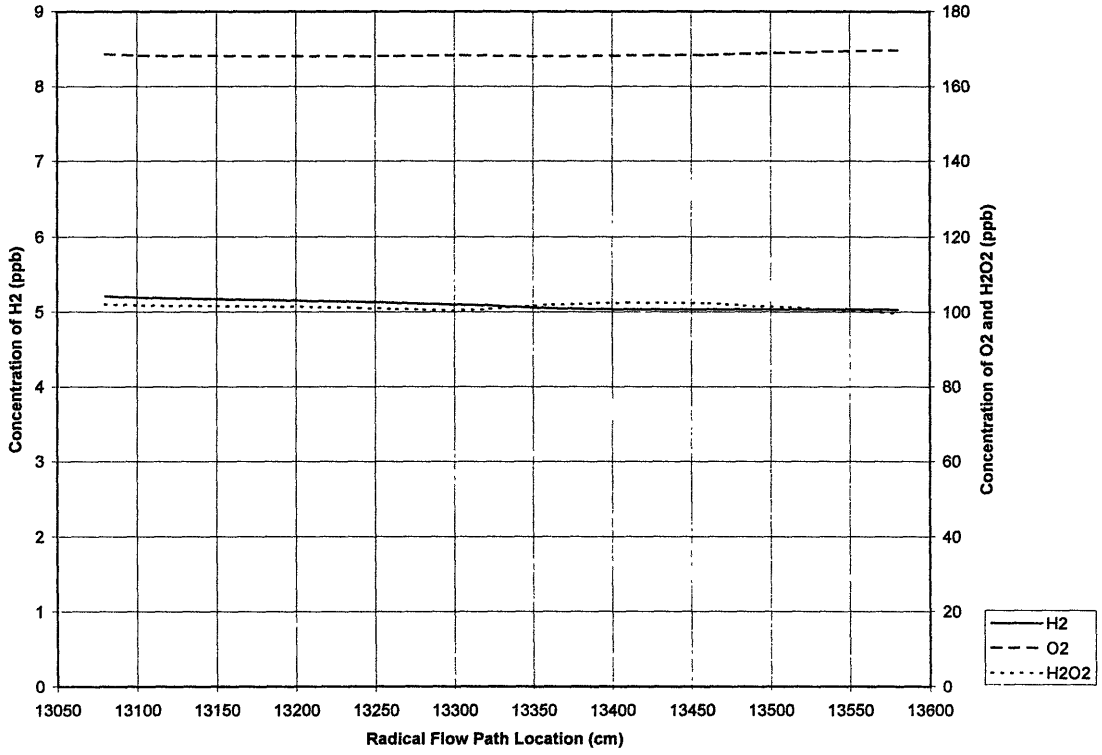

Figure 7.27 BWR-4 Jet Pump Concentrations

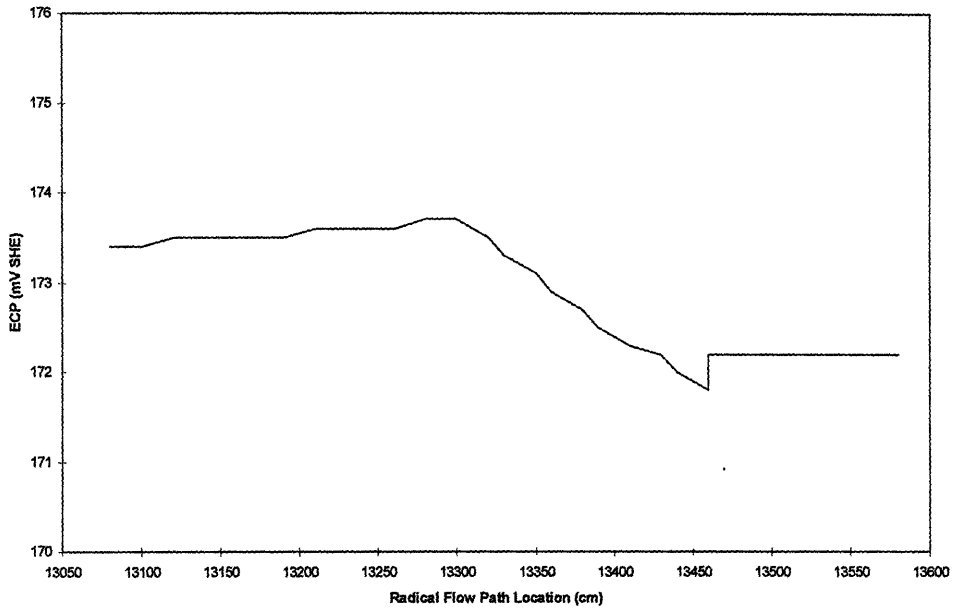

Figure 7.28 BWR-4 Jet Pump ECP

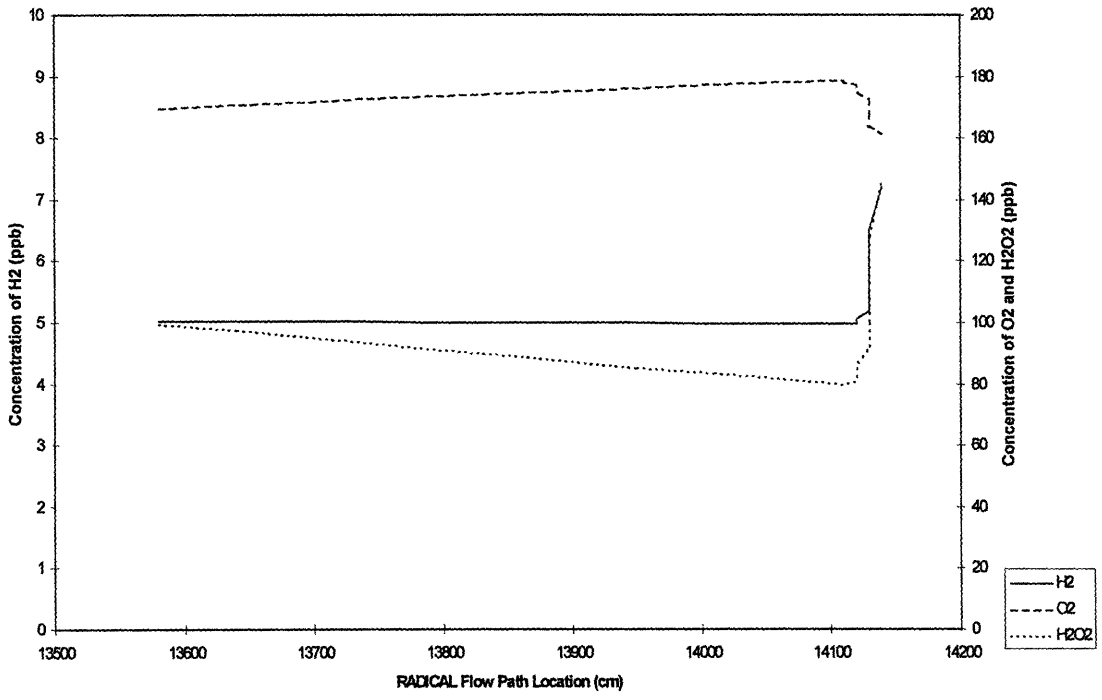

Figure 7.29 BWR-4 Lower Plenum Species Concentration

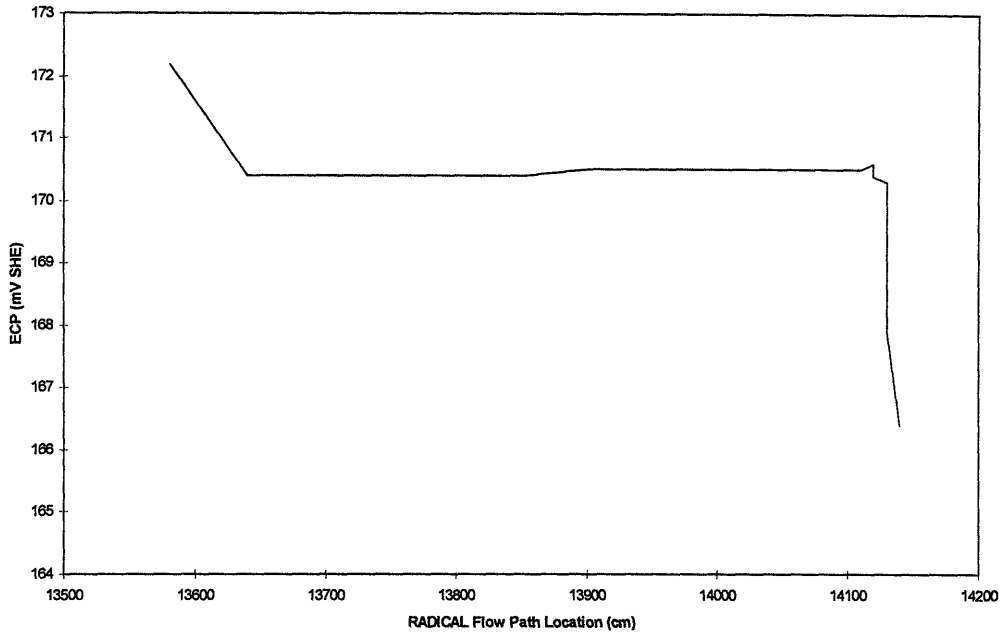

Figure 7.30 BWR-4 Lower Plenum ECP

7.3. Hydrogen Water Chemistry

Hydrogen water chemistry is the operating condition under which hydrogen is injected into the feedwater system in order to decrease the ECP. The purpose of the RADICAL code is to aid in selecting an appropriate injection level. To test the accuracy of the code, simulations were run for a typical BWR-3 and BWR-4 for a variety of injection levels. The results of these simulations are compared to MINITEST data from the comparable power plants. The MINITEST data are for a sample taken from the recirculation line. Comparing the recirculation line output to the test data results, Figures 7.31 and 7.34, show the predicted hydrogen values are slightly below the measured data and the predicted oxygen values are considerably below the measured values. This is probably due to decomposition of hydrogen peroxide in the measured samples prior to

measurements resulting in the higher oxygen values. To account for this phenomena a sample line component was added to the BWR system input file. The comparison of the sample line output and the MINITEST data is shown in Figures 7.32 and 7.35. Using the sample line model the concentration values better represent the measured values, for the BWR-4 the results are excellent for low hydrogen injection levels.

The effect of hydrogen injection on component ECP is shown in Figures 7.33 and 7.44 on a component by component basis. The ECP values drop regularly as injection levels are increased for most components. The components that maintain high ECP values are those with two-phase flow and restricted flow areas which result in high fluid velocities. These components are the core boiling, steam separators, and jet pump throat and diffuser. In addition the recirculation line components and jet pump tail also have high flow velocities. The rapid drops in these components only occur when oxidant concentrations drop to negligible values, less than 1 ppb. This may not be an actual effect as the ECP correlation used may not be valid at these higher velocities. The ECP at which IGSCC is no longer a major concern, -230 mV SHE, is denoted by a bold line for reference purposes.

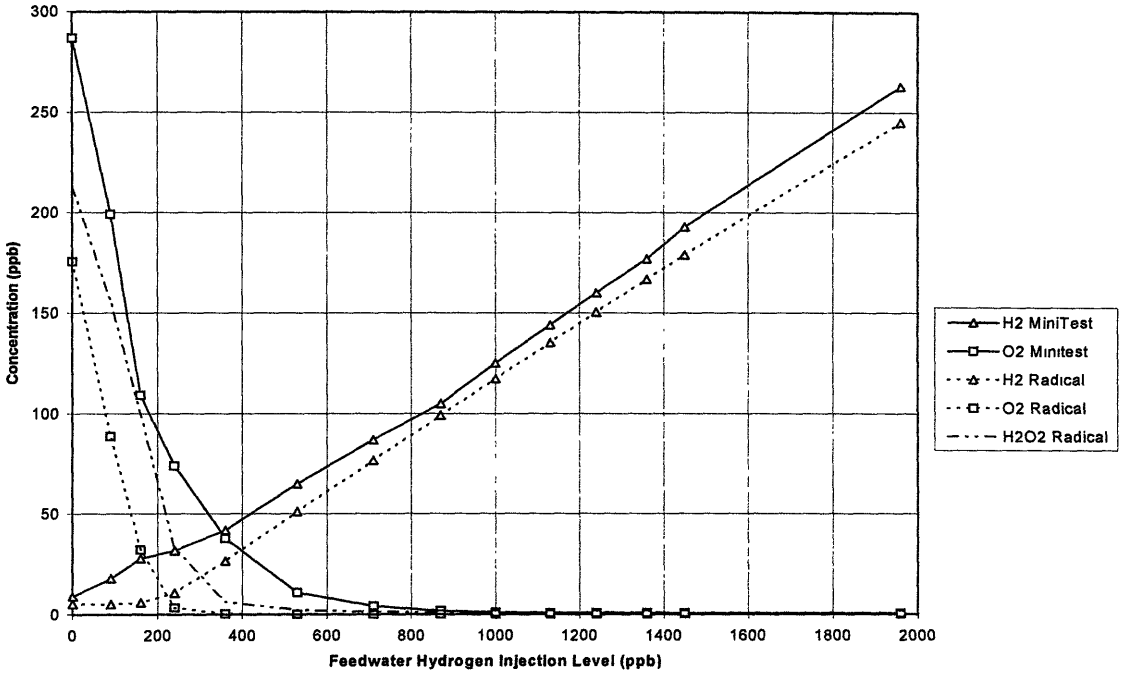

Figure 7.31 BWR-3 Comparison of MINITEST Data to Recirculation Line Concentrations

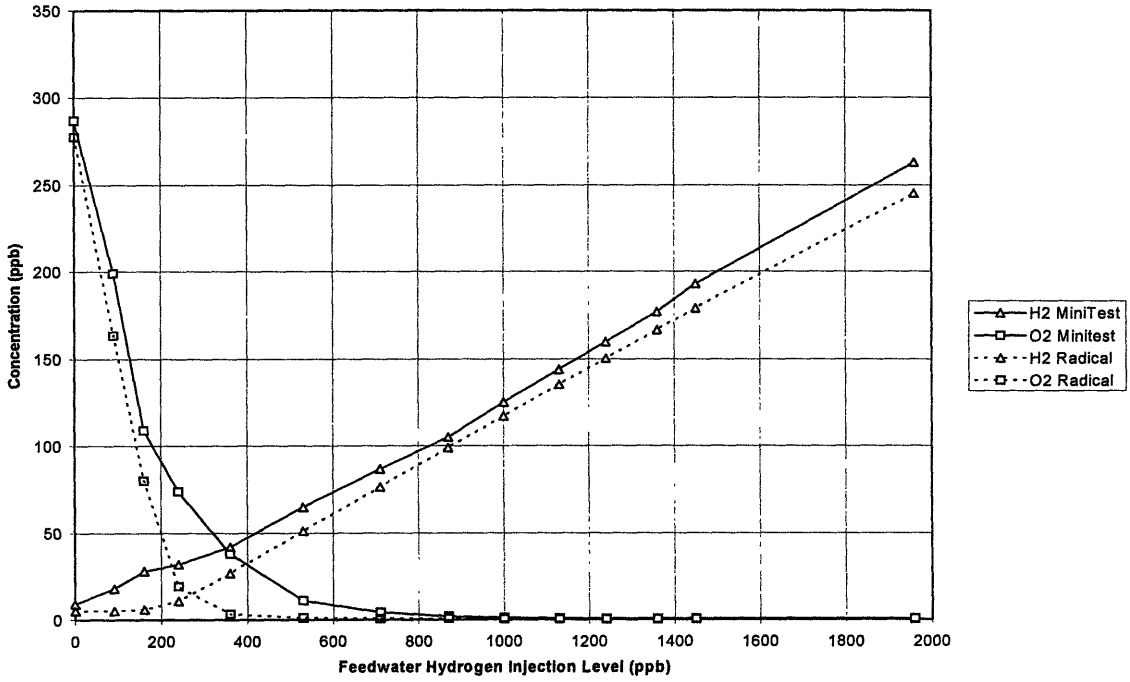

Figure 7.32 BWR-3 Comparison of MINITEST Data to Sample Line Concentrations

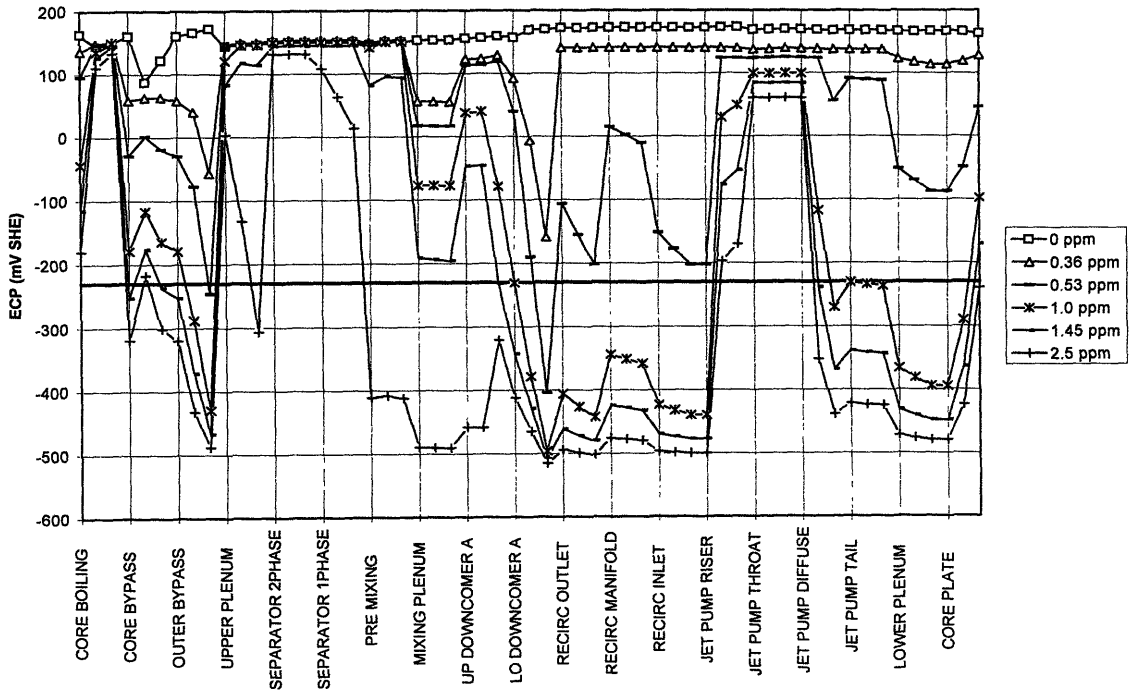

Figure 7.33 BWR-3 Component ECP for a Range of Hydrogen Injection Levels

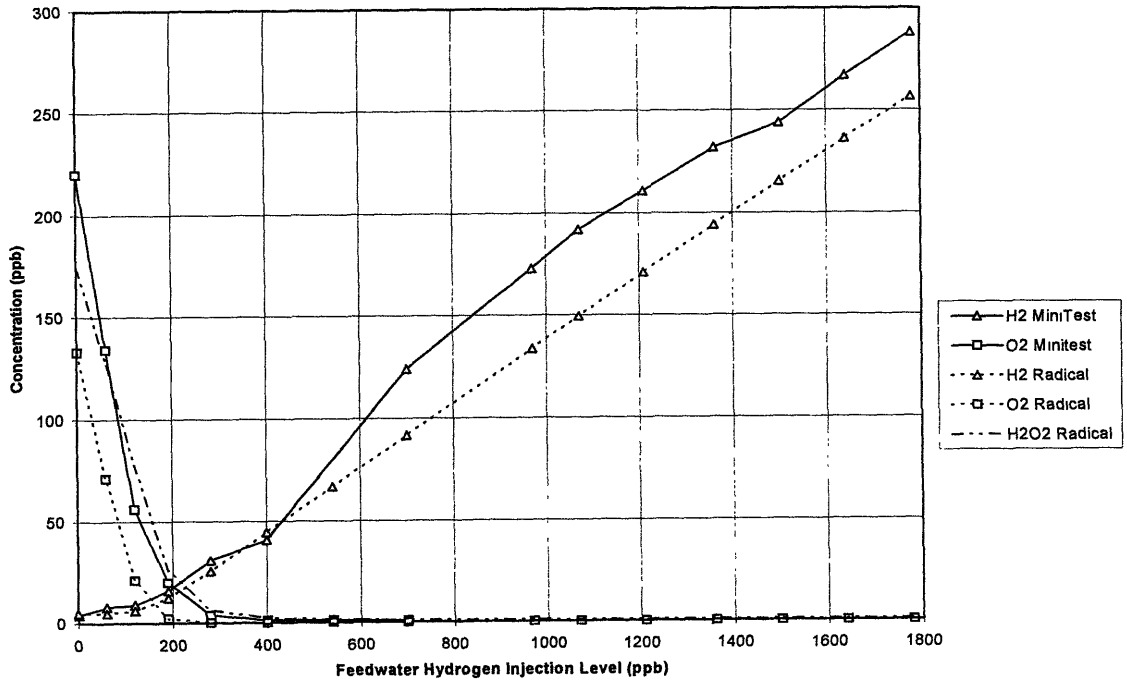

Figure 7.34 BWR-4 Comparison of MINITEST Data to Recirculation Line Concentrations

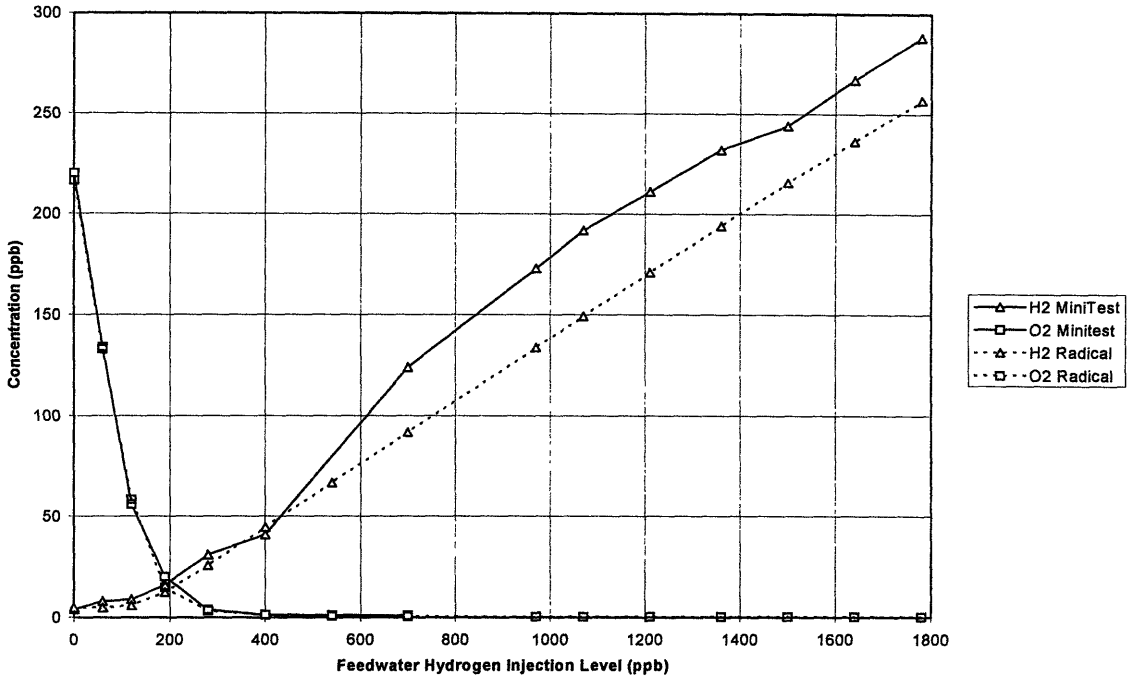

Figure 7.35 BWR-4 Comparison of MINITEST Data to Sample Line Concentrations

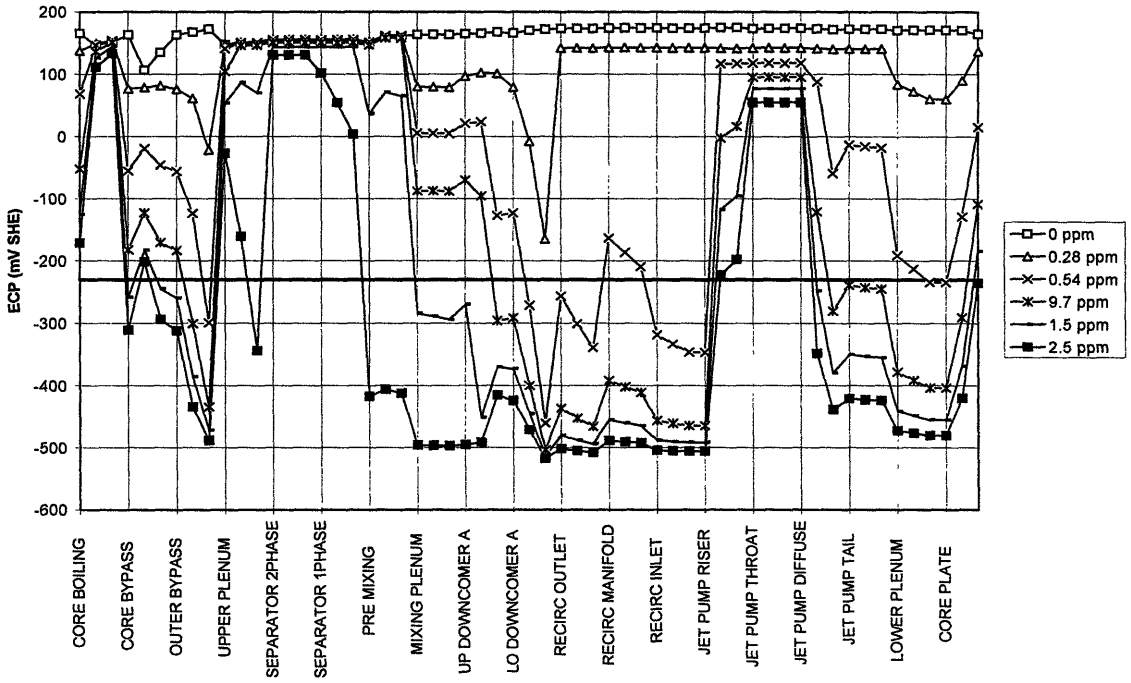

Figure 7.36 BWR-4 Component ECP for a Range of Hydrogen Injection Levels

7.4. Parametric Studies

Parametric studies were performed for two reasons. The first was to determine the variability of the calculated concentrations and ECP for the range of allowable operating conditions. The second was to aid in determining the degree of accuracy needed in characterizing the thermal hydraulic parameters needed for calculations. All parametric studies were conducted for the typical BWR-3 under normal water chemistry conditions.

7.4.1. Operating Conditions

These parametric studies were done for the range of allowable flow-power configurations to determine the what effect operating at partial power and or flow would have. Figure 7.37 shows the hydrogen concentration for this plant. The maximum value is located at the high flow-low power region. The concentration along the full power line is also the high edge with the concentration tapering off as the flow decreases. Figure 7.38 shows the oxygen concentrations at their maximum at the full power edge dropping off as the power decreases and also as the flow increases. Figure 7.39 shows the hydrogen peroxide having its maximum at midpower levels dropping slightly as power increases, but falling more rapidly as power drops. The peroxide also drops off as the flow rate decreases. However, the hydrogen still dominates the shape of the ECP surface as Figure 7.40 illustrates. The maximum ECP values are at the low flow-low power coordinates, dropping as either power or flow increase.

This ECP curve would suggest that when power is permitted to increase at flow levels 26% of maximum, it may be advisable to wait until the percentage of maximum flow reaches 50% or greater to avoid the higher corrosion potentials in this region.

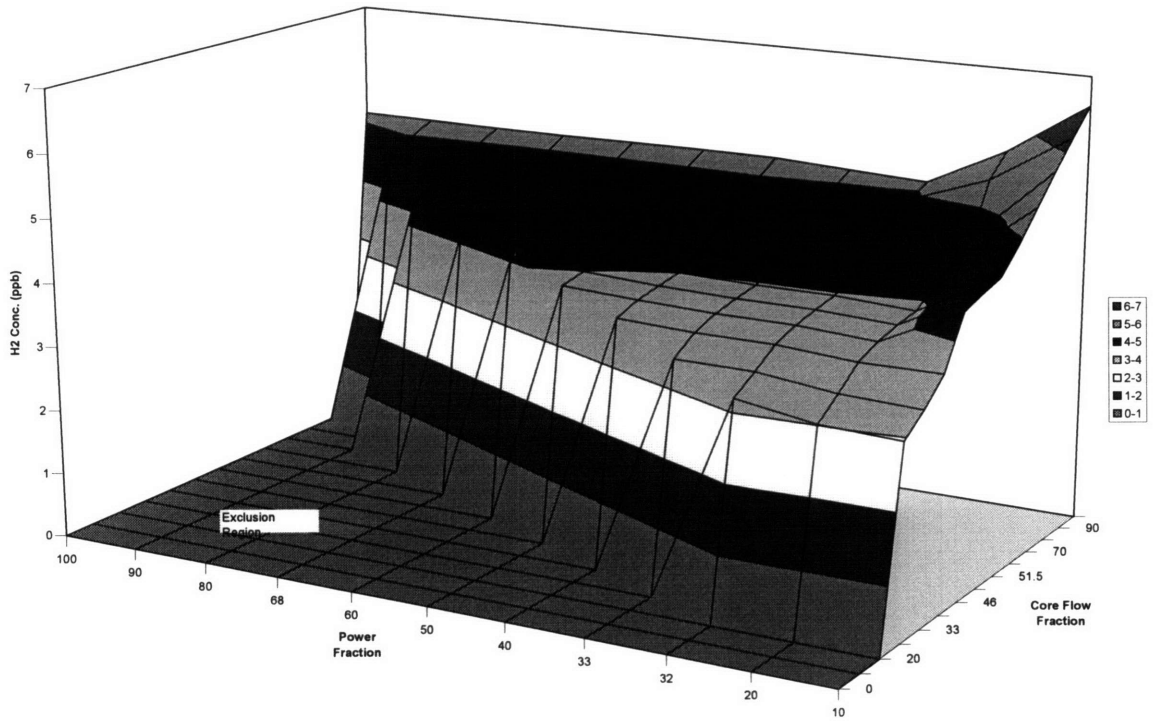

Figure 7.37 BWR-3 Hydrogen Concentration at the Recirculation Line Outlet for the Allowable Ranges of Flow and Power

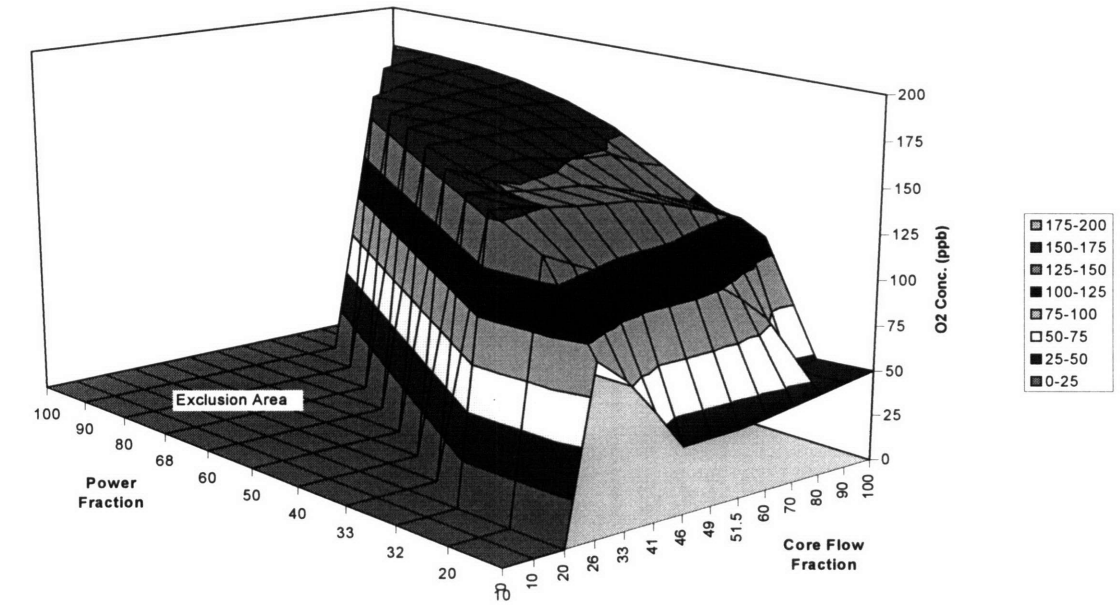

Figure 7.38 BWR-3 Oxygen Concentration at the Recirculation Line Outlet for the Allowable Ranges of Flow and Power

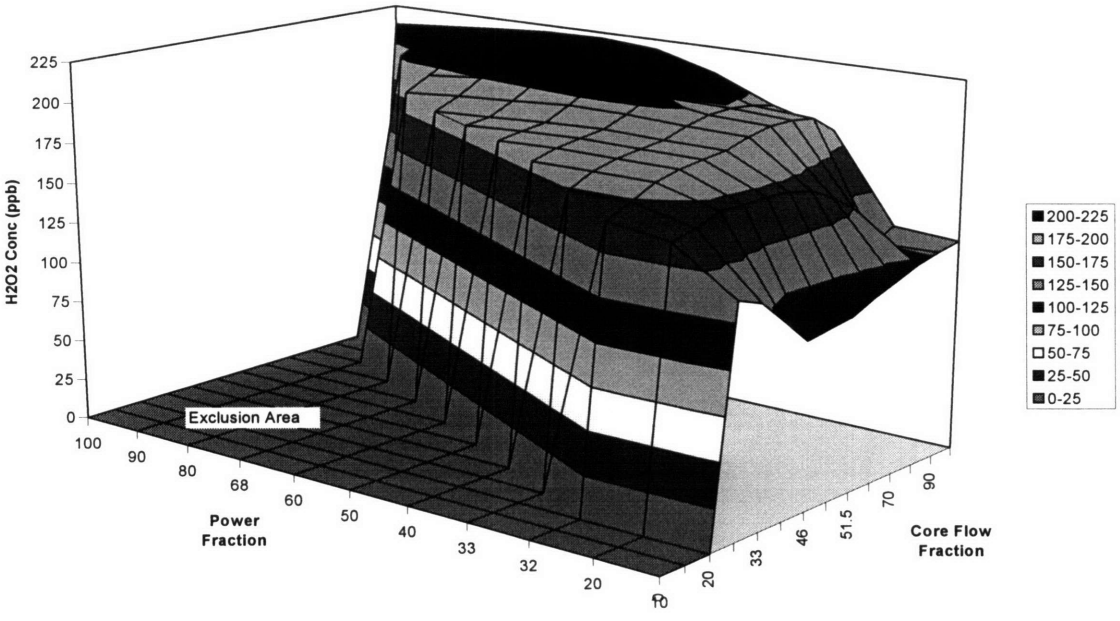

Figure 7.39 BWR-3 Hydrogen Peroxide Concentration at the Recirculation Line Outlet for the Allowable Ranges of Flow and Power

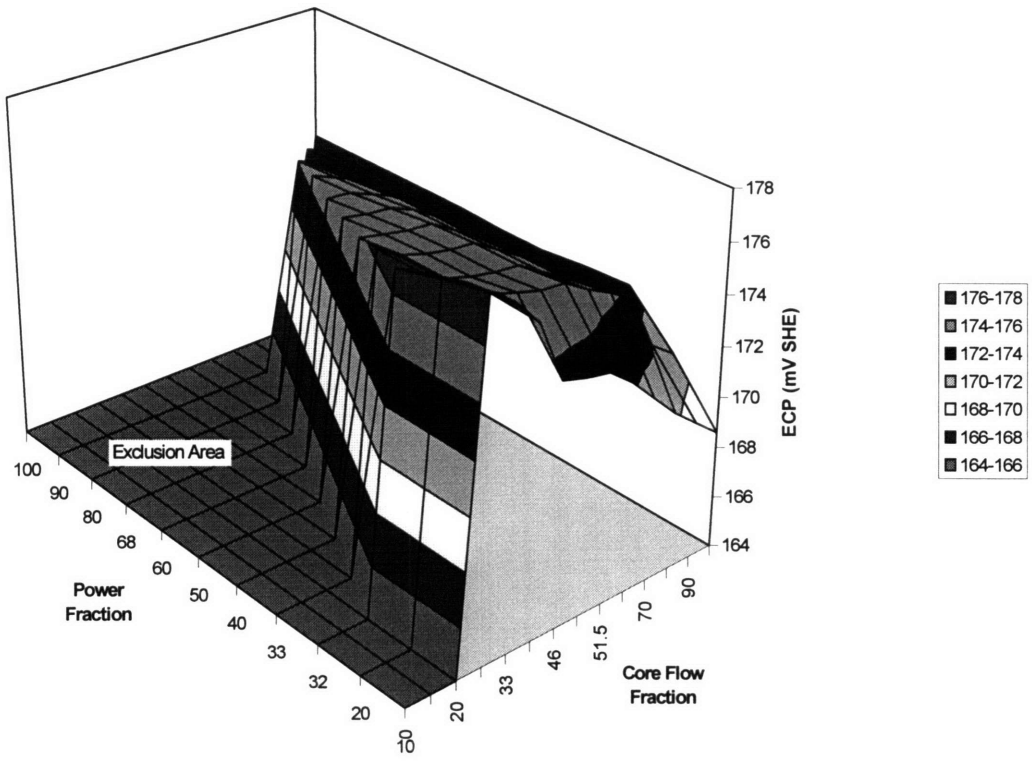

Figure 7.40 BWR-3 ECP at the Recirculation Line Outlet for the Allowable Ranges of Flow and Power

7.4.2. Parameter Accuracy

The parameters examined for their effect on concentration were hydraulic diameters, radiation levels, and thermodynamic parameters.

The first set of studies were to determine the effect of hydraulic diameters on the hydrogen concentrations obtained at the sample line for comparison with the MINITEST data. The effect of each components and its effect is shown on Figures 7.41 and 7.42. These show that with the exception of the bypass regions in the core, components having hydraulic diameters below 30 cm have the most importance in correctly determining the hydrogen concentration.

Figures 7.43 and 7.44 show the same holds true for the oxygen concentrations, with the steam separator components having the largest effect.

In addition the effect these diameters have on the concentrations within the component is of concern to accurately model local water chemistry not just that measured at the sample line. Figures 7.45 and 7.46 show the effect hydraulic diameter has on the exit hydrogen concentration for the component whose diameter is adjusted. Here the main components effected are the core boiling and core bypass regions. The boiling region hydraulic diameter is well characterized for reactor performance reasons. However the bypass region still needs to be better characterized. Figures 7.47 and 7.48 show that all components except the 2-phase region of the steam separator, core plate, and upper plenum have an effect on the oxygen concentrations when the hydraulic diameter decreases below 25 cm. Figures 7.49 and 7.50 show that a hydraulic diameter below 25 cm for all compoents has a significant impact on hydrogen peroxide concentrations. These studies suggest that while only the separator regions have a major effect on the sample line output, all component diameters need to be well characterized to accurately determine local chemistry.

Other parametric studies for thermodynamic properties include:

Total mass flow rate	Figure 7.51
Flow fraction through boiling channel	Figure 7.52
Flow fraction along core periphery with boiling flow constant	Figure 7.53
Flow fraction through recirc system	Figure 7.54

Core inlet temperature	Figure 7.55
Feedwater inlet temperature	Figure 7.56
System operating pressure	Figure 7.57

Varying these parameters show only a slight effect on the concentrations in the component where they have the greatest thermodynamic effect.

The only remaining studies are for the operating power level and the radiation dose levels independent of each other, Figure 7.58 and 7.59 correspondingly. These show that both have a major effect on concentrations and should be modeled carefully. The effect that these have acting together is shown as the 100% flow line for the operational parametric studies in Section 7.4.1.

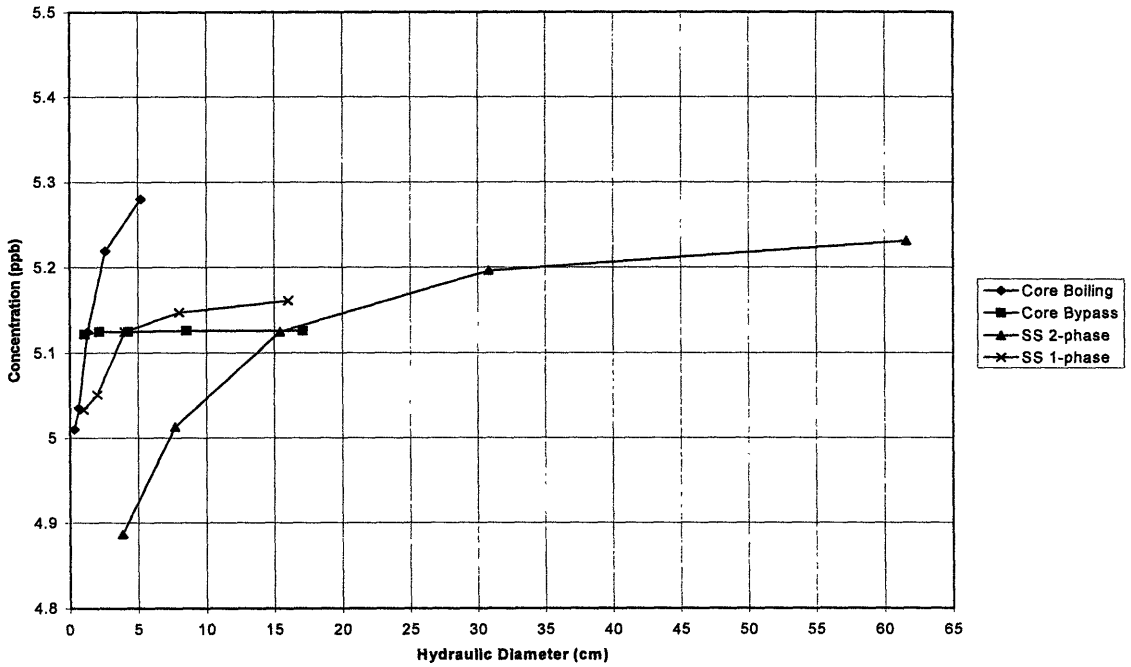

Figure 7.41 Effect of Component Hydraulic Diameter on Sample Line Hydrogen Concentration

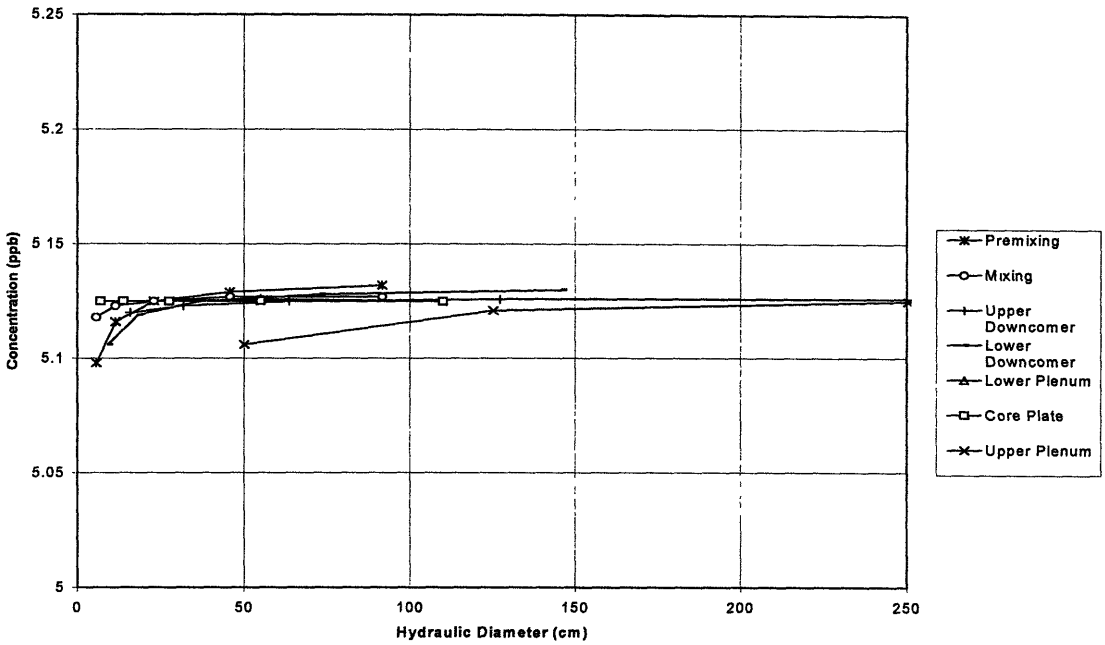

Figure 7.42 Effect of Component Hydraulic Diameter on Sample Line Hydrogen Concentration

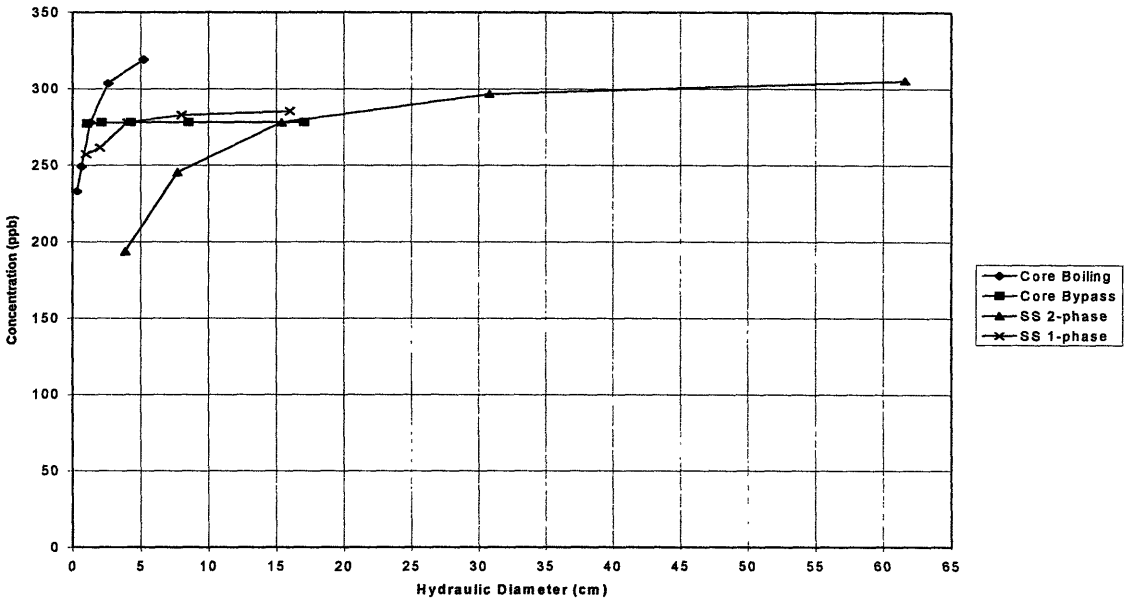

Figure 7.43 Effect of Component Hydraulic Diameter on Sample Line Oxygen Concentration

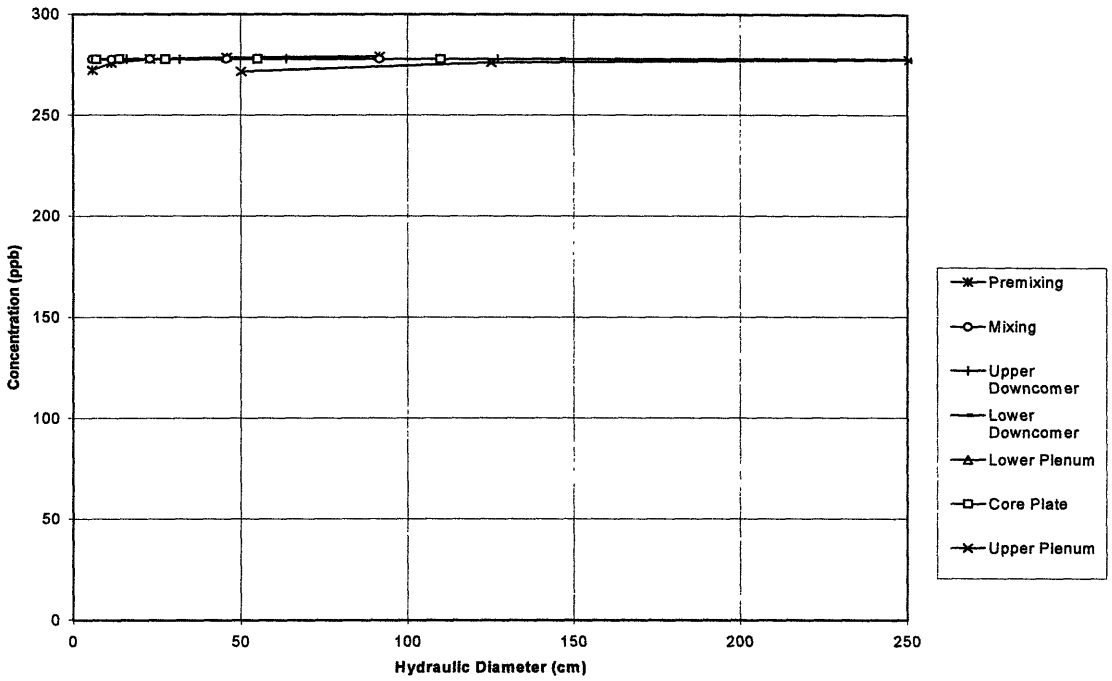

Figure 7.44 Effect of Component Hydraulic Diameter on Sample Line Oxygen Concentration

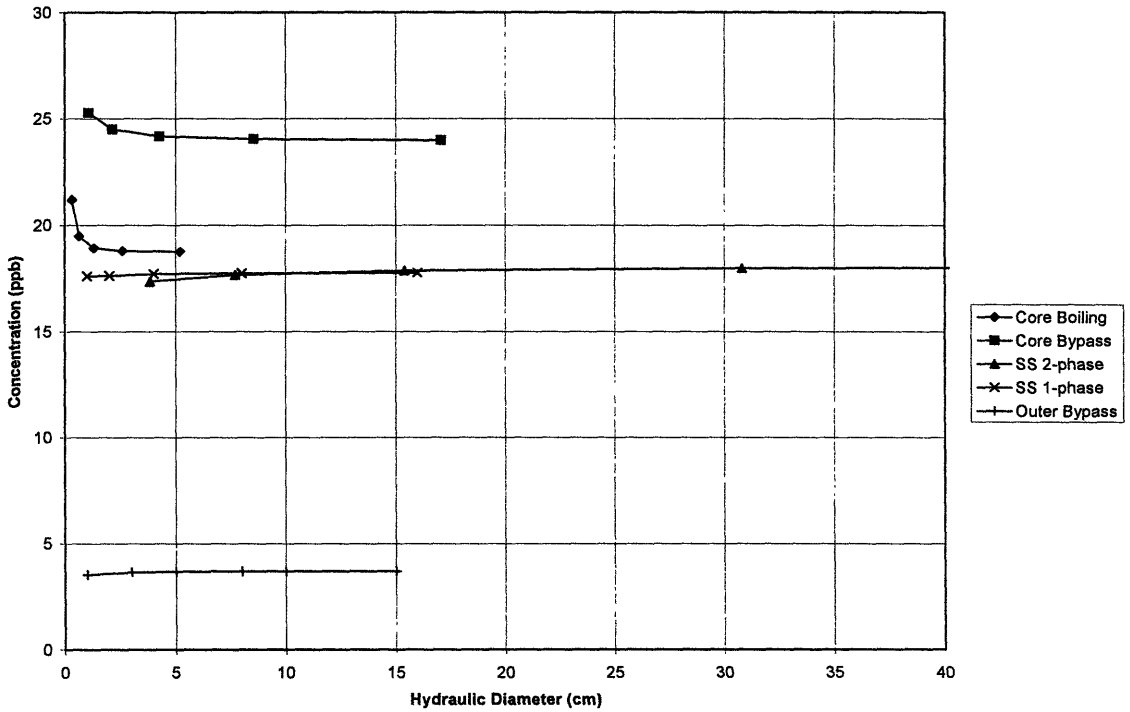

Figure 7.45 Effect of Component Hydraulic Diameter on Component Exit Hydrogen Concentration

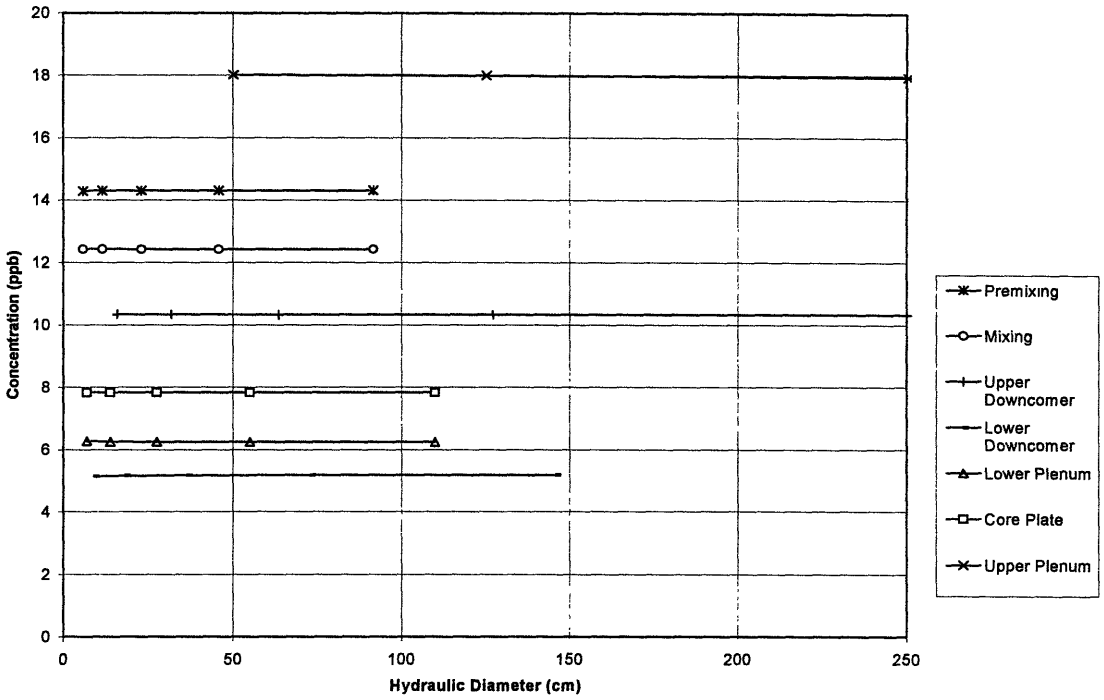

Figure 7.46 Effect of Component Hydraulic Diameter on Component Exit Hydrogen Concentration

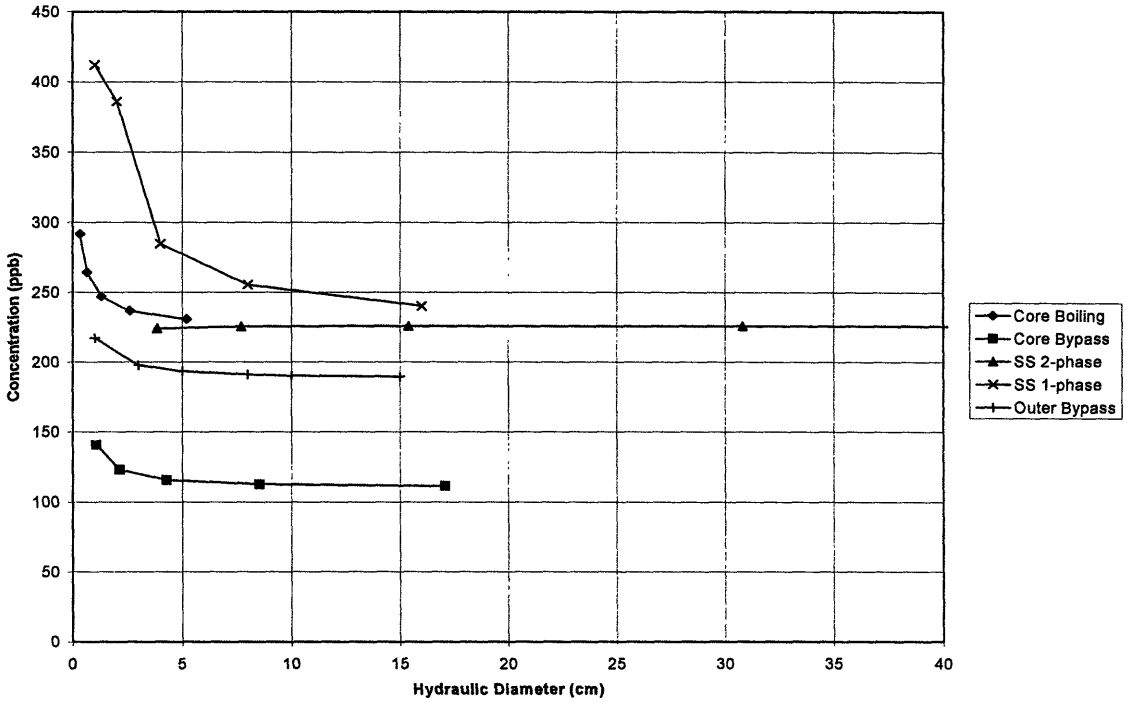

Figure 7.47 Effect of Component Hydraulic Diameter on Component Exit Oxygen Concentration

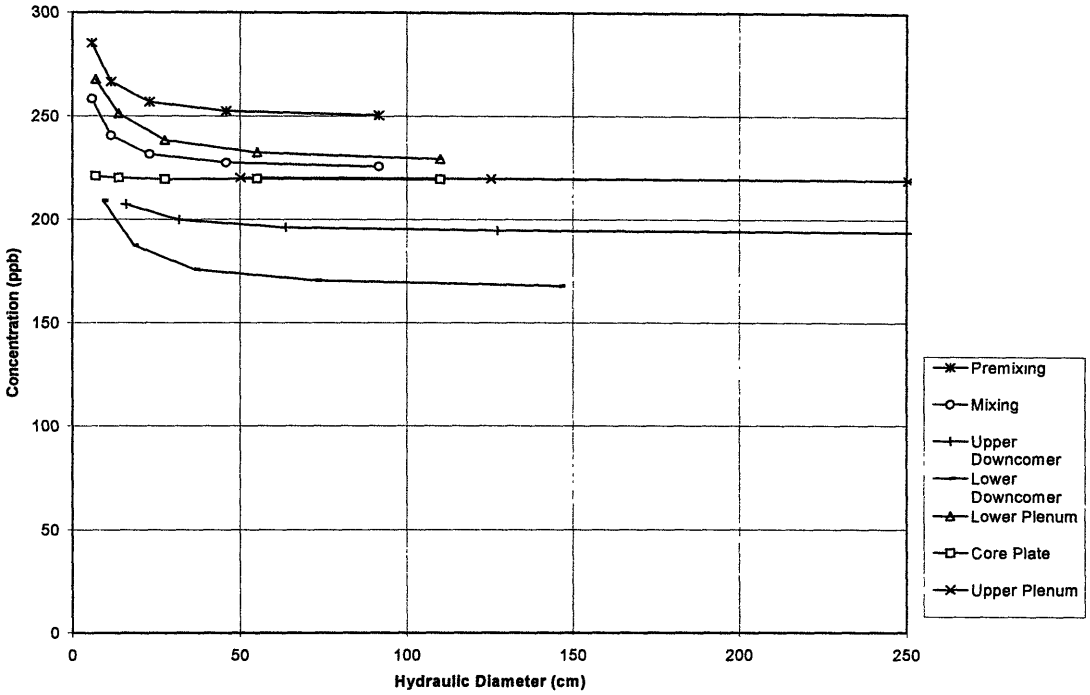

Figure 7.48 Effect of Component Hydraulic Diameter on Component Exit Oxygen Concentration

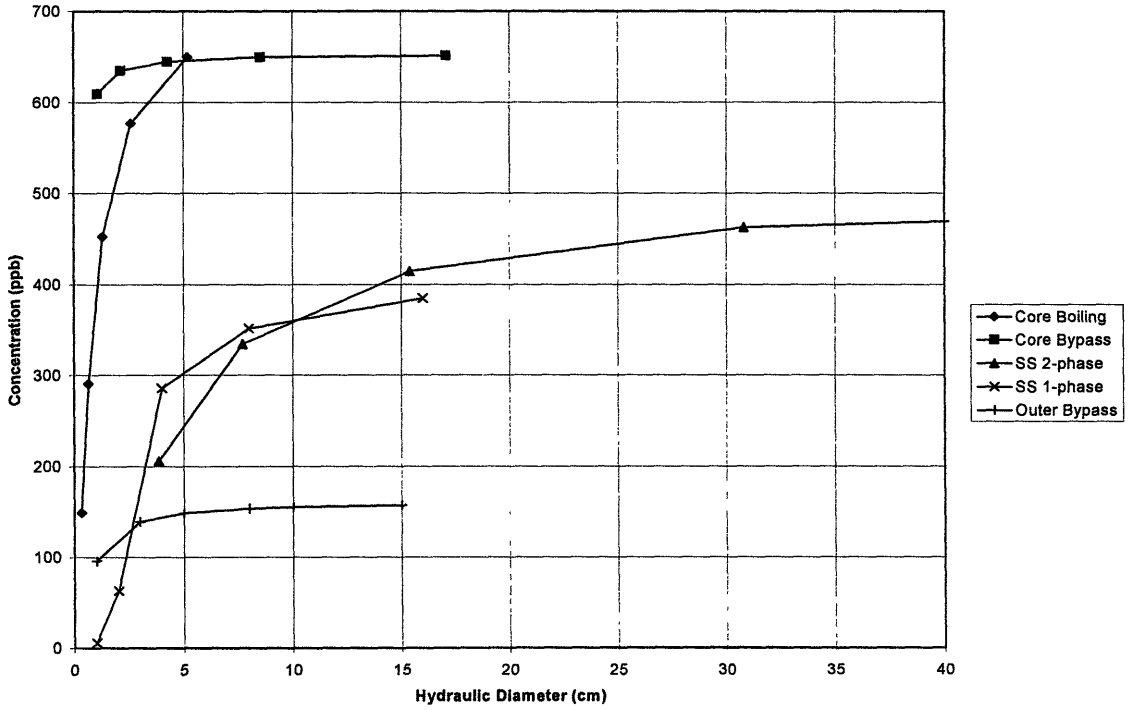

Figure 7.49 Effect of Component Hydraulic Diameter on Component Exit Hydrogen Peroxide Concentration

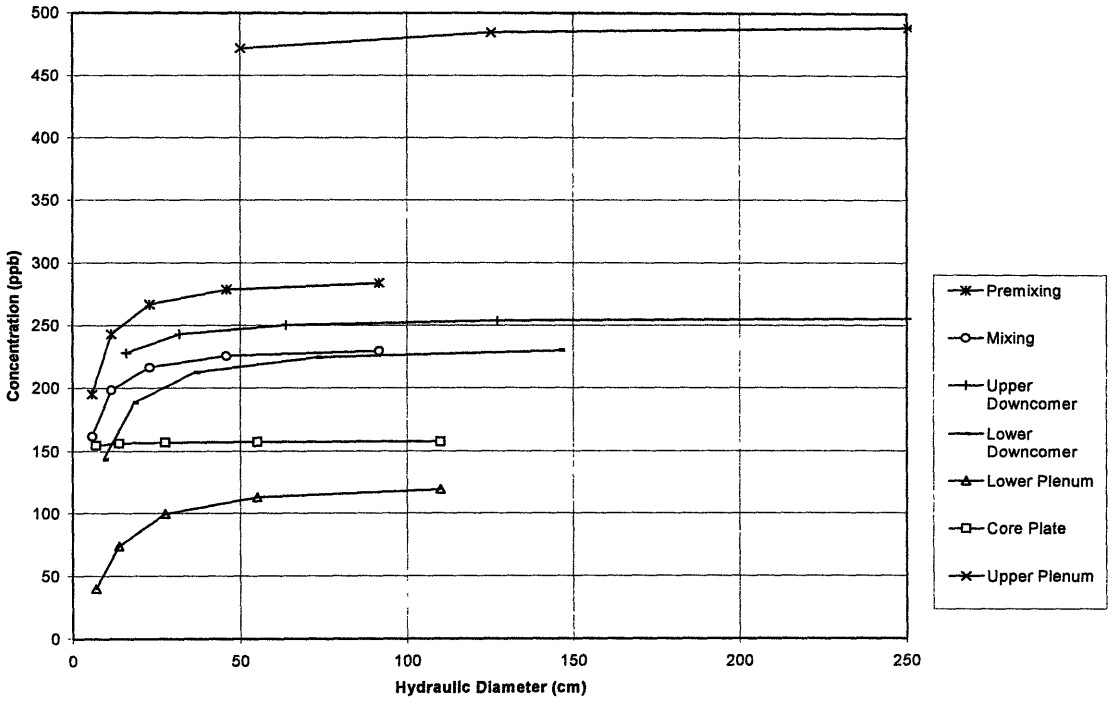

Figure 7.50 Effect of Component Hydraulic Diameter on Component Exit Hydrogen Peroxide Concentration

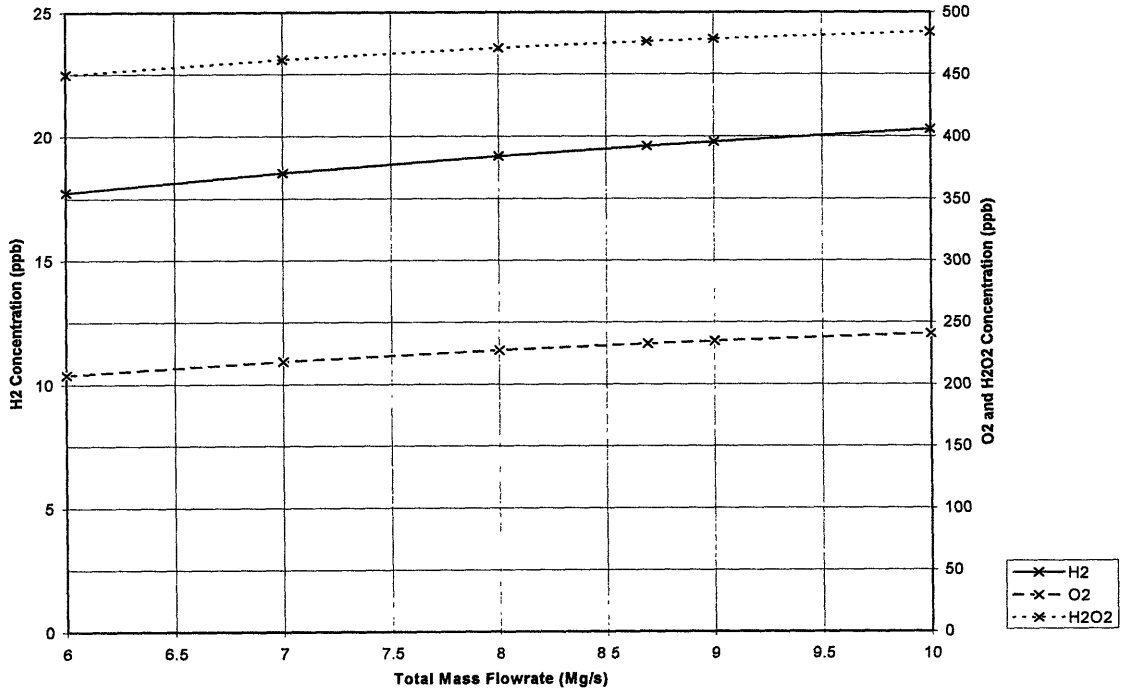

Figure 7.51 Effect of Total Mass Flow Rate on Species Concentration In the Upper Plenum

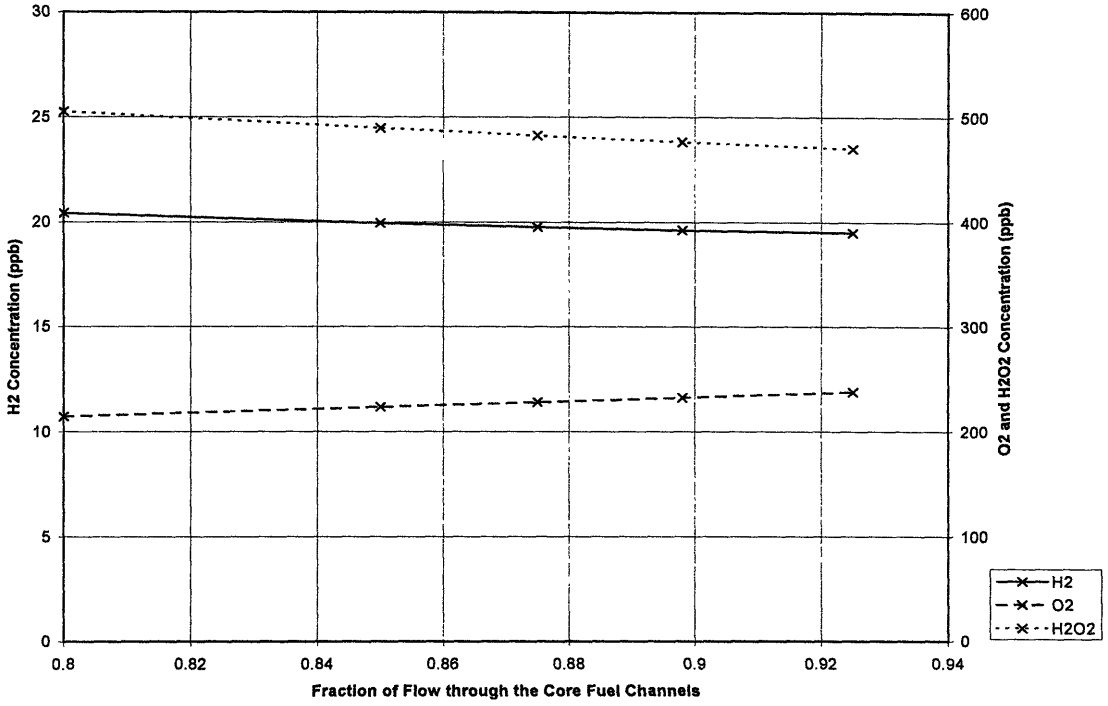

Figure 7.52 Effect of Flow Fraction through Boiling Channels on Species Concentrations in the Upper Plenum

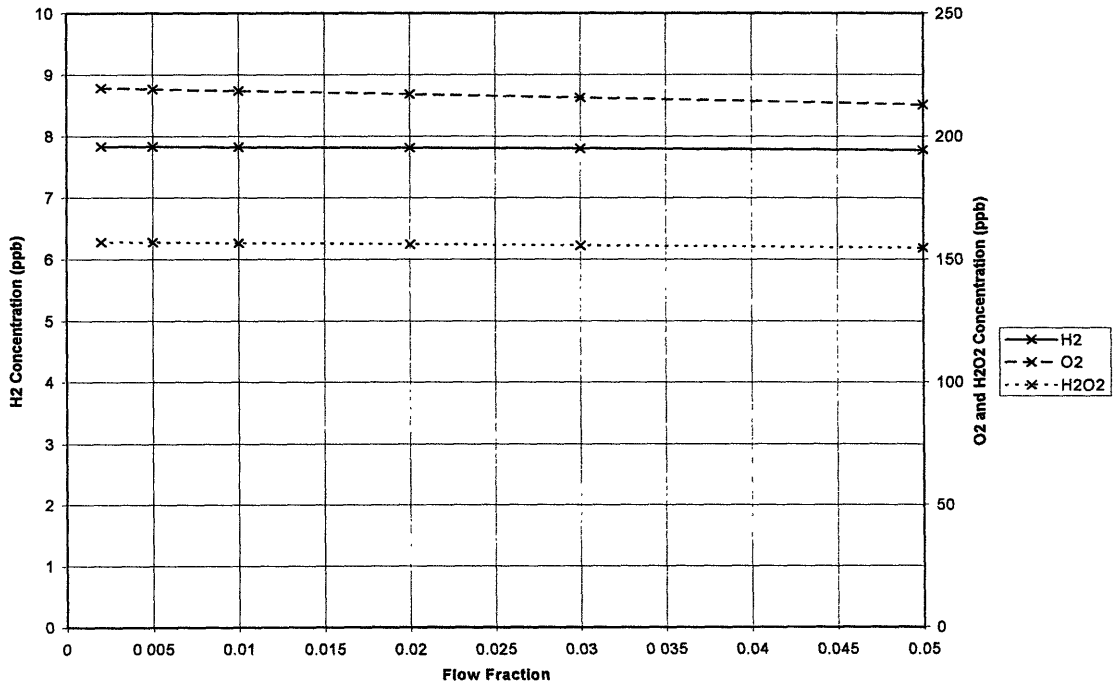

Figure 7.53 Effect of Flow Fraction Along Core Periphery on Species Concentrations in the Upper Plenum

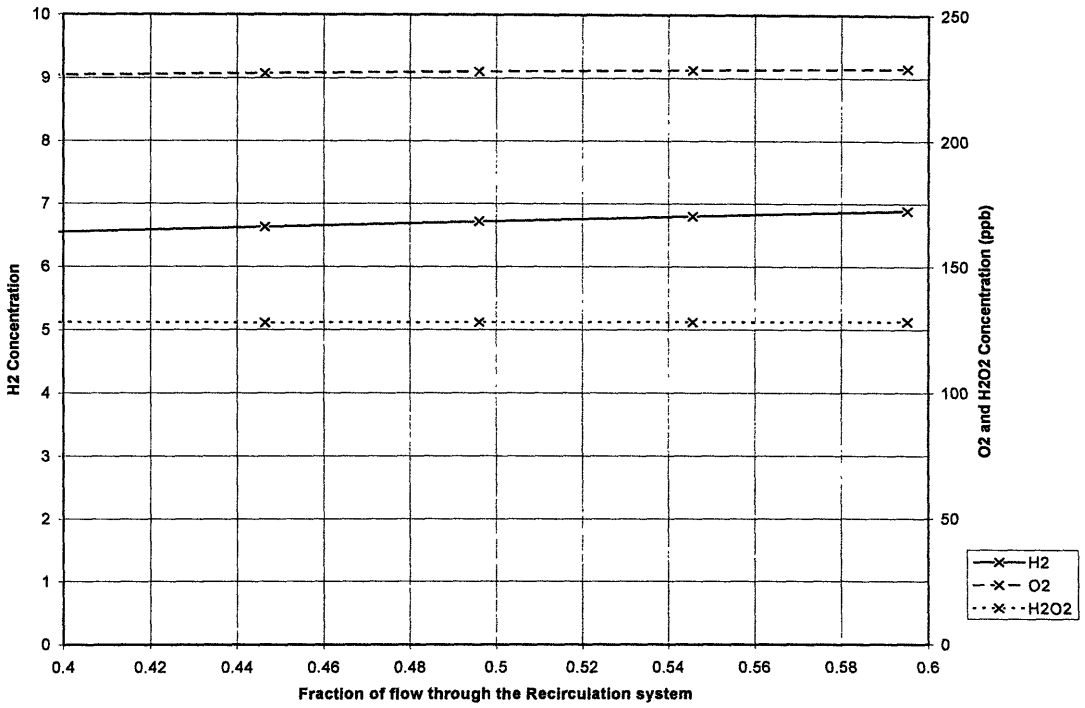

Figure 7.54 Effect of Flow Fraction Through the Recirculation System on Species Concentration in the Jet Pump Throat

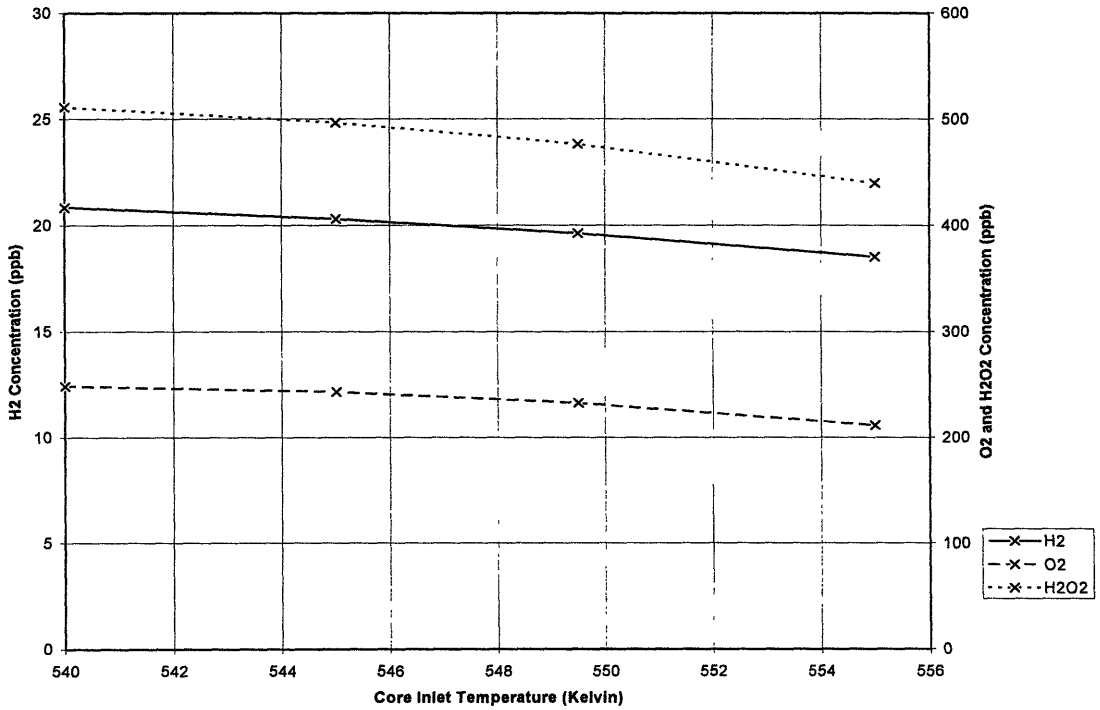

Figure 7.55 Effect of Core Inlet Temperature on Species Concentrations in the Upper Plenum

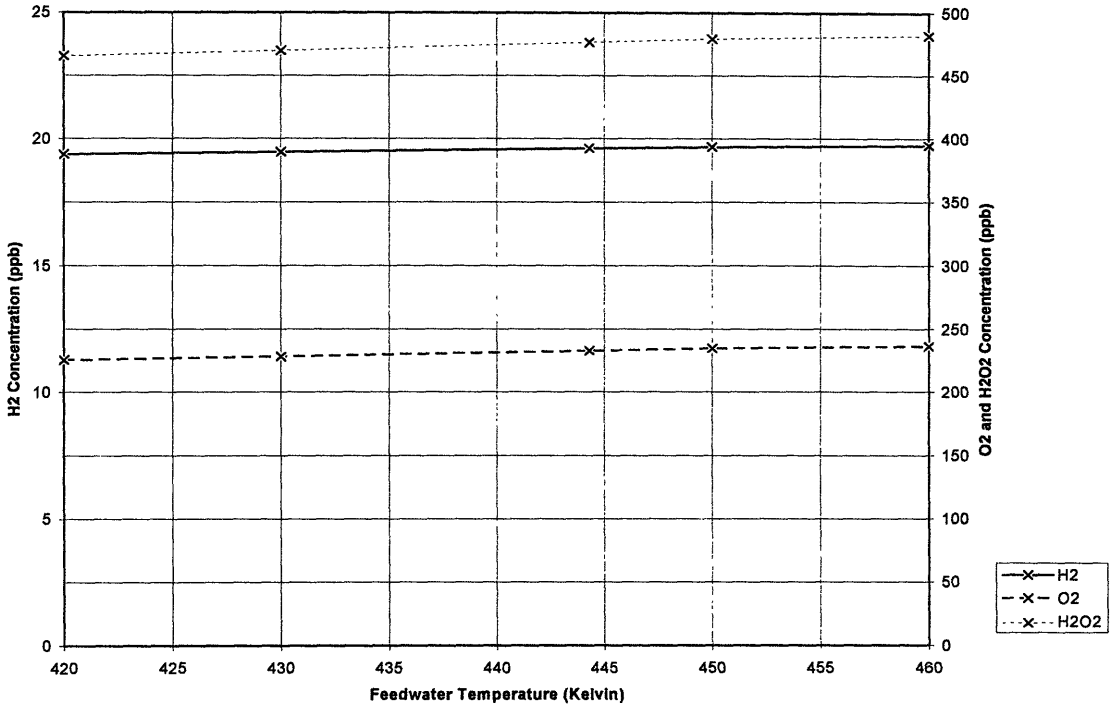

Figure 7.56 Effect of Feedwater Temperature on Species Concentrations in the Upper Plenum

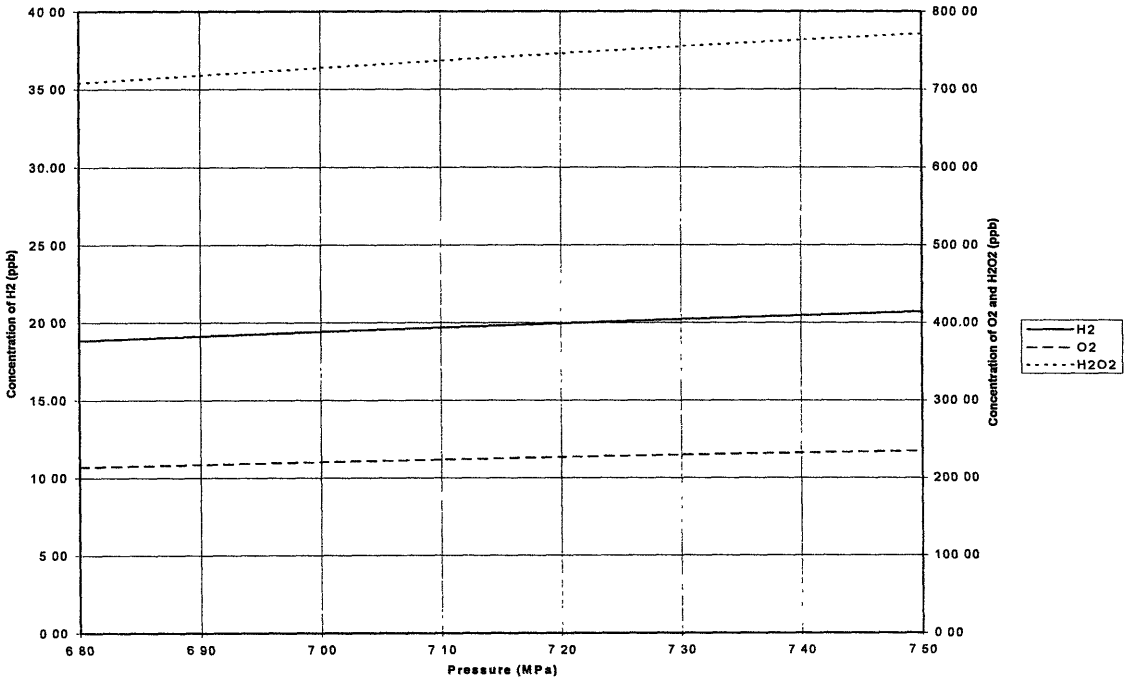

Figure 7.57 Effect of System Operating Pressure on Species Concentrations in the Upper Plenum

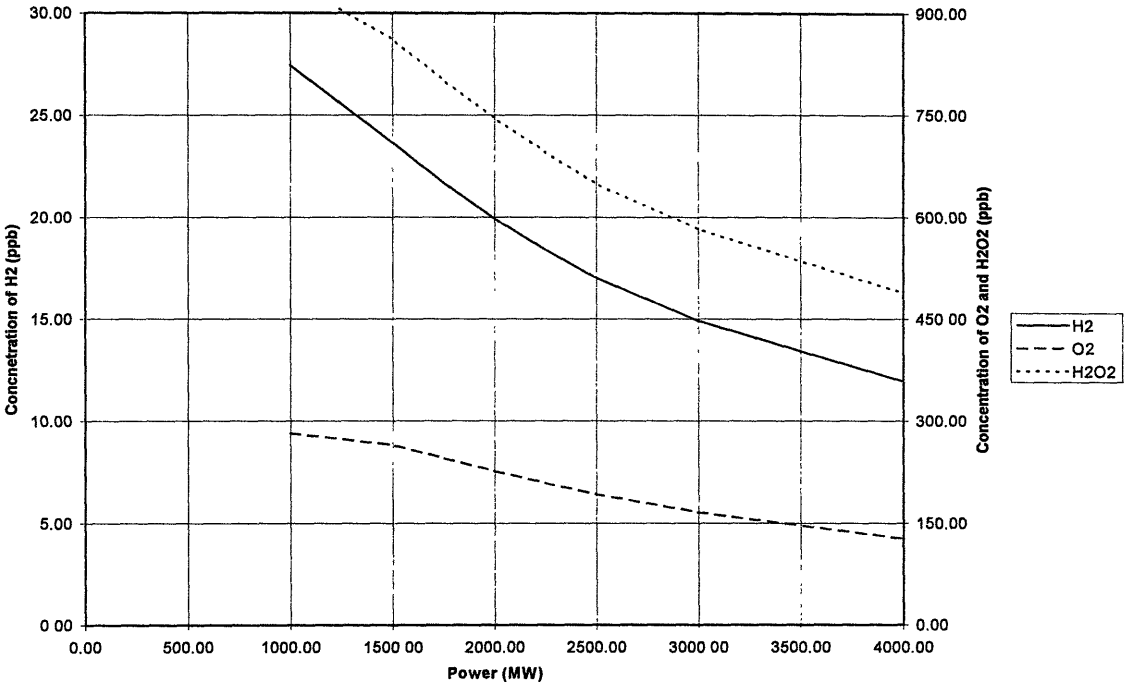

Figure 7.58 Effect of Average Power Level on Species Concentration At the Recirculation Line Outlet

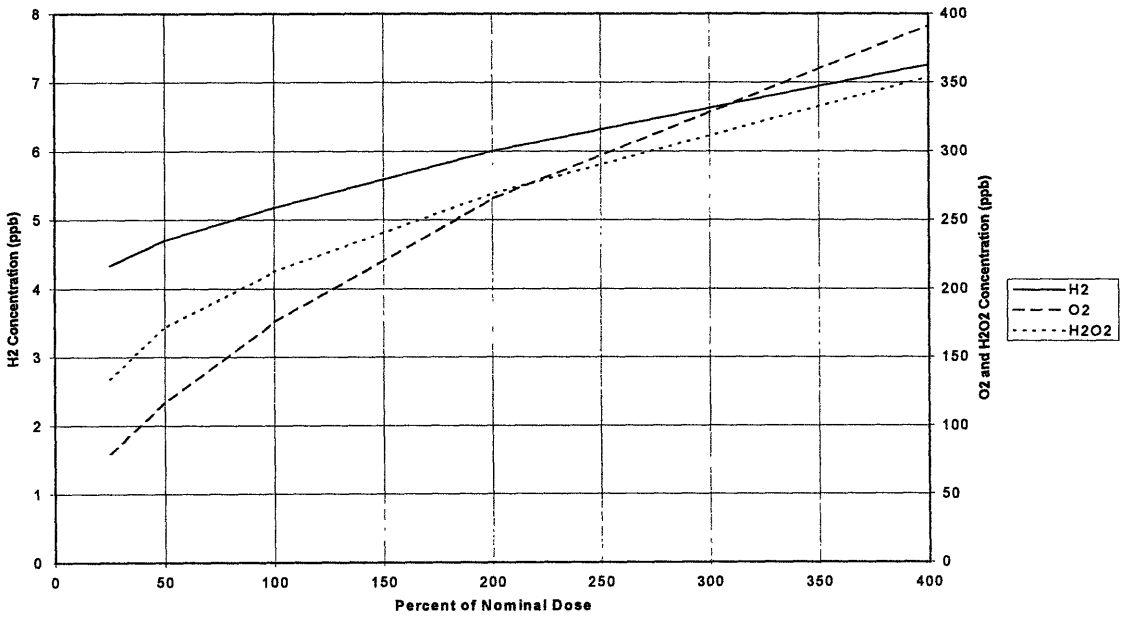

Figure 7.59 Effect of Average Radiation Dose on Species Concentration at the Recirculation Line Outlet

8. Conclusions

The ability to incorporate variable cross-sectional area component modeling has been successfully integrated into the RADICAL model. In conjunction with the new model of the BWR primary coolant flow path, the model provides results comparable to measured data for a typical BWR-3 and BWR-4. Also an improved ECP correlation has been included to predict the corrosive environment due to hydrogen, oxygen, and hydrogen peroxide concentrations as well as the effect of velocity.

8.1. Significance of Results

The major result of the current simulation is that the measured data from a typical BWR-3 and BWR-4 can be closely predicted by the RADICAL model. The simulation also demonstrates the necessity of modeling the sample lines to accurately compare the measured and calculated data. This is due to the effect hydrogen decomposition has on the oxygen levels in the sample lines.

The new ECP correlation demonstrates that controlling oxygen alone below 20 ppb will not drop the ECP below -230 mV SHE. Hydrogen peroxide also plays a similar role. In addition both need to be eliminated in high flow regions to have the desired effect. However caution must be used in the last case as the flow velocities in two-phase flow regions and in the recirculation system exceed the maximum velocity limitation for the correlation.

For parametric studies an important result is that regions of the permissible range of power-flow combination, based on thermal-hydraulic parameters, may

need to be avoided to minimize the ECP during power build-up and coast-down. These regions are the combination of low-flow, less than 50%, and low power, also below 50%. Instead flow should be raised first to above 50% with power up then occurring. These results are based on normal water chemistry and should be repeated for hydrogen water chemistry cases to ensure the phenomena remains similar.

Parametric studies to determine the accuracy of input parameters show that of the thermodynamic parameters power and doserate potentially have the largest impact and should be modeled accurately. In addition hydraulic diameters were studied. While only the steam separator component diameters had the most effect on the sample concentrations, all components with hydraulic diameters less than approximately 25 cm can have a substantial effect on the local concentrations and need to be accurately represented to model the ECP along the entire flow path.

8.2. Future Work

The development of the RADICAL model is an on-going process, with the modifications described in this thesis another step in improving its versatility and accuracy.

In addition to the continual revisions in estimating g-values, chemical reaction rate constants, and mass transfer coefficients between phases suggested by Chun [1990], the following are being considered to improve the code.

- Detailed characterization of plant geometry, In the simulation runs many approximations and assumptions were made regarding the geometry of the primary coolant path. The use of plant computerized drawings to characterize cross-sectional areas, hydraulic diameters and component lengths would eliminate much of the uncertainty in the concentrations and ECP due to the assumptions made.
- Update the variable area model, The current variable area model is a linear interpolation between exit and entrance areas. With the detailed information mentioned above a more complex model of the area and differential area can be made similar to that used to characterize dose and power profiles. This will allow characterization of the flow velocity within individual components, such as the downcomer, having a complex geometry
- Develop an ECP correlation for high velocity regions, the majority of the primary coolant flows at velocities at or above the highest recommended by the correlation developers. Some regions of interest such as the recirculation line has a velocity at least double the maximum recommended. This is vital to ensure that hydrogen injection levels necessary to reduce the ECP to below -230 mV (SHE) without unnecessarily increasing doserates in the turbine buildings.
- Develop data sets detailing power, gamma dose, and neutron flux for a variety of operating conditions. A mentioned previously these parameters have a large impact on calculated concentrations. Also mentioned was

how allowable power-flow operating combinations should be avoided to minimize ECP during start-up and coast-down. Well characterized data will improve knowledge of what power-flow combinations to avoid, as well as improving estimation of hydrogen injection levels. These data sets should consider the range of operating power levels for the various stages of the fuel burnup cycle to manage hydrogen water chemistry throughout the plant life cycle.

Many of the above recommendations are currently ongoing or soon to be started. RADICAL is currently being modified with a graphical user interface with input and output files accessed via a database. With these modifications in place RADICAL can become a more effective tool in hydrogen water chemistry management and corrosion control.

References

Burns, W. G. and P. B. Moore, *Radiat. Eff.*, **30**, 233, 1976.

Burns, W. G. and P. B. Moore, "Radiation Enhancement of Zircaloy Corrosion in Boiling Water Systems: A Study of Simulated Radiation Chemical Kinetics", *Proc. Int. Conf. Water Chemistry of* Nuclear *Reactor Systems*, Bournemouth, England, pp. 281, BNES, 1978.

Carver, M. B., D. V. Hanley, and K. R. Chaplin, "MAKSIMA-CHEMIST: A Program for Mass Action Kinetics Simulation by Automatic Chemical Equation Manipulation and Integration Using Stiff Techniques", AECL-6413, Atomic Energy of Canada, Ltd., Chalk River Laboratories, 1979.

Christensen, H.; "Radiolysis of Reactor Water", Proc. *1988 JAIF Conf. on Water Chemistry of Nuclear Power Plant, April 19-22, 1988, Tokyo, Vol.2.*, p. 505, 1988

Cowan, R. L. et al.; "Recent Developments in BWR Water Chemistry Control", *2nd International Topical Meeting on Nuclear Power Plant Themal Hydraulics and Operations,* Tokyo, Japan, 1986.

"Final Safety Analysis Report Volume !, Pilgrim Nuclear Power Station", Boston Edison Company, 1970.

Chun, J. H.; "Modeling of BWR Water Chemistry", SM thesis, Nuclear Engineering, MIT, Cambridge, MA, 1990.

Chun, J. H. and R. Ballinger; "Modeling of BWR Water Chemistry and Thermal Hydraulics for Oxidizing Species Concentrations, Volume 1: Theory Manual", EPRI Report Tr-103366-V1, 1993.

Elliot, A. J., D. C. Ouellette, and D. R> McCracken; "G-Values for Gamma-Irradiated Water as a Function of Temperature", to be published (journal unknown), 1990.

Fontana, M. G.; Corrosion Engineering 3rd Ed., McGraw-Hill, Inc., New York, 1986.

Hindmarsh, A. C.; "ODEPACK, A Systematized Collection of ODE Solvers", *Scientific Computing*, R. Stepleman, ed., North-Holland Publishing Co., pp.55-64, 1983.

Ibe, E. and S. Uchida; "Computer Simulation for Water Radiolysis in BWRs", *Trans. Am. Nucl. Soc.*, **41**, p. 242, 1982

Ibe, E. and S. Uchida; "Analytical Evaluation of Water Radiolysis in BWRS", *Proc. 3rd Int. Conf. Water Chemistry of Nuclear Reactor Systems, No. 7*, BNES, Bournemouth, England, October 17-21, 1983.

Ibe, E. and S. Uchida; "Evaluation of the Yields from the Radiolysis of Water in Boiling Water Reactors by Neutron and Gamma Radiation", *Nuclear Science and Enginnering,* **85**, pp. 339-349, 1983.

Ibe, E. and S. Uchida; "A Water Radiolysis Model in a Circulating Flow System with a Boiling Region and Its Application to Hydrogen Alternative Water Chemistry of Boiling Water Reactors", *Nuclear Science and Engineering*, **89**, pp. 140-157, 1985.

Ibe, E. and S. Uchida; "Radiolytic Aspects in Boiling Water Reactor Primary Systems: Results from Numerical Simulations and Statistical Regression Analyses", *Nuclear Science and Engineering*, **89**, pp. 330-350, 1985.

Ibe, E. et al.; " Numerical Techniques for Quantitative Evaluation of Chemical Reaction Systems with Volatile Species and Their Application to Water Radiolysis in BWRs" *J. Nuclear Materials*, **130**, pp. 45-50, 1985

Ibe, E. et. al.; "Theoretical Model Analyses for Effects of Hydrogen Injection on Radiolysis of Coolant Water in BWR", *J. Nuclear Science and Technology*, **23**[1], pp. 11-28, January 1986.

Ibe, E. et al.; "Radiolytic Environments in Boiling Water Reactor Cores", *J. Nuclear Science and Technology*, **26**[8], pp. 760-769, August 1989.

Ibe, E. et al.; "Parameter identification of wate radiolysis in BWR primary systems", *Proc.* 5th *Int. Conf. Water Chemistry of Nuclear Reactor Systems, No. 5* BNES, Bournemouth, England, 1989

Jones, D. A.; Principles and Prevention of Corrosion, Prentice-Hall, Inc., New Jersey, 1992

Kent, M. C. and H. E. Sims; "The Yeild of γ-radiolysis Products from Water at Temperatures up to 270°C", AEA Reactor Services Repot AEA-RS-2302, 1992

Lin C. C.et. al.; "Prediction of Electrochemical Corrosion Potentials in BWR Primary Systems Volume 2. Development of Stainless Steel ECP Models", EPRI Report-Draft, 1994

Macdononald, D. D.; " Viability of Hydrogen Water Chemistry for Protecting In-Vessel Components of Boiling Water Reactors", Corrosion, 48, pp. 194-205, March 1992.

Romeo, G. et. al., "BWR Vessels and Internals Project, Modeling Hydrogen Water Chemistry for BWR Applications-New Results (BWRVIP-13)", EPRI Report TR-106068, 1995.

Ruiz, C. P. et. al.; "Modeling Hydrogen Water Chemistry for BWR Applications", EPRI Report NP-6386, 1989.

Ruiz, C. P.;"Modeling Hydrogen Water Chemistry for BWR Applications Program Description and Status, Presentation, February, 1993.

Schmidt, K. H.; "Computer Program for the Kinetic Treatment of Radiation-Induced Simultaneous Chemical Reactions: A Revised Version in FORTRAN-IV", ANL-7693, Argonee National Laboratory, 1970

Simonson, S.; "Modeling of Radiation Effects of Nuclear Waste Package Materials", PhD Thesis, Nuclear Engineering, MIT, Cambridge, MA, 1988.

Takagi, J. et al.; "Evaluation of Corrosion Environment in BWR Priamry Circuit by Water Radiolysis Model", *Proceedings - JAIF International Conference on Water Chemistry in Nuclear Power Plants*, *Vol. 2*, pp. 517-522, 1988

Todreas, N. E. and M. S. Kazimi; Nuclear Systems I, Hemisphere Publishing Corp., New York, 1990.

Uchida, S. et al.; "Applicationof Hydrogen Water Chemistry to Moderate Corrosive Circumstances Around the Reactor Pressure Vessel Bottom of Boiling Water Reactors", *Nuclear Technology*, **110** [2], pp. 250-257, May 1995.

Yeh, T. K. and D. D. Macdonald; "Modeling the Development of Damage in BWR Primary Coolant Circuits", *Proc. Seventh International Symposium on Environmental Degradation of Materials in Nuclear Power Systems - Water Reactors Volume 2*, NACE International, Breckenridge, CO, 1995.

Appendix A Radical User's Manual

The RADICAL User's Manual consists of four sections. The first describes the syntax required by the code. The second defines the parameters and gives details on their usage by the code. The third instructs which variables should be defined in the input file for a variety of available thermo-hydraulic data and desired output form. The final section explains the calculation of many of the physical parameters.

1. Input File Creation

There are two main sections of the input file. The first contains parameters which are common to the entire system. The second contains information which is specific to individual components within the system. Parameters are grouped by function into several categories. These groups are then read into the program one at a time using the NAMELIST method.

NAMELIST defines a set of parameters under a group name; in the input file each group begins with an ampersand ('&') immediately, i.e. no spaces, before the group name. The parameters begin in the next line. Parameter names are listed in any order, followed by an equals sign ('=') and the parameter value. All parameters for a group need not be listed, If a parameter is not specified it will default to a previous declared value. The end of the group is signaled by a forward slash ('/'). On a final formatting note all lines must begin with the first character in the second column.

For the loop parameters there are six groups, twelve groups for the component parameters. All loop parameter groups must be included even if no

parameters are declared, in this case the group name is followed by a space and the forward slash. Some component groups are conditional and identified as such, along with the circumstances for which they can be omitted.

2. Parameters

Loop Parameters

Group Name: FileName

This group is used to specify the unique files, to which the results of the RADICAL code will be written.

Variable	Data Type or (Units)	Default Value	Description
OutFile	Character	'radical.out'	Desired output file name and path, e.g. C:\radical\test.out. This file holds output in an easily read format.
PlotFile	Character	'radical.plo'	Desired plotting output file name and path, e.g. C:\radical\test.plo. This file holds tab delimited output for easy importation into graphing programs.
InjectFile	Character	'radical.hwc'	Desired HWC output file name and path, e.g. C:\radical\test.hwc. This file is also configured for graphing programs.

Group Name: Control

This group specifies the models to be used in calculating concentrations. Also controls input and output format and sensitivity calculations.

Variable	Data Type or (Units)	Default Value	Description
NCycle	integer	1000	The number of loop calculation iterations desired for the answer: to be used if no convergence criteria is specified.
NodeStart	integer	1	The component node at which calculations begin. Initial concentrations must be specified for this node in the component parameters.

FlowRateTot	(g/second)	1.d0	Mass flow rate of the primary coolant.
PlotOut	logical	true	Is a flag for the generation of a plot file, true generates the file, false does not.
SensLoop	logical	false	Is a flag used for sensitivity analysis, false overrides the flag for component sensitivity analysis, SensComp, resulting in no calculation of sensitivity for any components.
SurfLoop	logical	true	Is a flag used to control if hydrogen peroxide surface decomposition effects will be accounted for in the program. True considers the effect, false neglects the effect. False also overrides the SurfComp flags.
Debug	logical	false	Is a flag used to control debugging routines in the code. There is a number of them in the code, each with its' own flag. false means no use of the debugging routine
CalcConc	logical	true	Is a flag used to control whether the radiolysis calculations are to be done. These calculations are omitted for one cycle in order to calculate the heat balance.
CycleOut	logical	all false except cycle 1 and last cycle	Is a flag used to control output at each cycle. If true then the information for that cycle is included in the output file.
CyclePlot	logical	true	Is a flag used to control output at each cycle. If true then the information for that cycle is included in the plot file.
HeatBalance	logical	true	Is a flag used to control whether a thermodynamic heat balance is to be calculated for the cycle or not. true, i.e. the balance is calculated.
HeatBalComp	character	blank	The component at which the heat balance is calculated. This must be specified in the input file. The recommended component is 'premixing.'
ConcInMode	character	ppb	Is the units used for inputted concentrations.
ConcOutMode	character	ppb	Is the units used for outputted concentrations.

ConvComp	character	blank	Is the component at which convergence is tested. the default value is blank. If convergence testing is desired this must be declared in the input file. The recommended component is 'CoreBoiling.'
ConvMin	(%/100))	0.001	Is the convergence criteria.
ConvSpecies	character	blank	Are the chemical species for which convergence is checked. The default values are blank and must be declared in the input file. The recommended species are 'O2', 'H2', and 'H2O2.'
PowerFactor	real	1.0	Is a multiplication factor applied to PowerAvg, GammaAvg, and NeutAvg to allow for the power to be scaled in together easily for parametric studies.
DoseFactor	real	1.0	Is a multiplication factor applied to GammaAvg and NeutAvg to allow the total dose to be scaled easily for parametric studies.
GammaFactor	real	1.0	Is a multiplication factor applied to GammaAvg to allow the gamma dose to be scaled easily for parametric studies in conjunction with DoseFactor the same can be done for neutron dose.
CalcInject	logical	false	Is the flag used to specify whether hydrogen water chemistry will be calculated. The default value is false, i.e. no calculation. True will repeat the cycle calculations for a range of hydrogen injection rates.
Inject Species	character	hydrogen	is the chemical species which is being injected into the feedwater. Previously only hydrogen was allowed now other species can be injected as well.
InjectComp	character	blank	is the component at which hydrogen is injected. The default value is blank and must be declared in the input file if HWC is to be calculated, typically 'feedwater.'
Inject	(ppb)	-1.d0	Is the level of hydrogen injection in ppb. A range of values can be entered here to simulate a different injection levels.

Group Name: RXControl

This group describes the parameters for chemical reactions.

Variable	Data Type or (Units)	Default Value	Description
NSurfRX	integer	0	Is the number of surface reactions in the reaction set.
TempRef	(Kelvin)	298.0	Is the reference temperature to be used in the Arrhenius calculation for chemical reactions.
WaterImplicit	logical	none	Flag which declares whether water is implicitly (true) or explicitly (false) declared.

Group Name: GValue

This group describes the generation of chemical species due to radiation, and must be entered in the input file. These parameters are read line by line, therefore all data pertaining to a reaction set must be contained on one line. These g-values are based on water chemistry research and will be maintained by the code originators. A listing of possible chemical reactions is located in the file GValue.Lib, (in process of being created).

Variable	Data Type or (Units)	Default Value	Description
SpeciesName	character	none	Is an array of the names of the chemical species being generated.
GGammma	(#species/ 100ev)	none	Is the G-Value for production of this species in number of molecules per 100eV due to gamma radiation.
GNeut	(#species/ 100ev)	none	Is the G-Value for production of this species in number of molecules per 100eV due to neutron radiation.
MolWt	(g/mole)	none	Is the molecular weight of the chemical species.

A partial example of this input section is shown below, for the full set view the sample input file attached in the next section:

```
$GValue
 H2      0.800      0.88      2.000D+00
 O2                           3.200D+01
 H2O2    0.28       0.99      3.400D+01
 O2G                          3.200D+01
$End OF GValue
```

Group Name: Reaction

This group describes the chemical reactions which occur in the reactor water. These parameters are read line by line, therefore all data pertaining to a reaction set must be contained on one line. These reactions are based on water chemistry research and will be maintained by the code originators. A listing of possible chemical reactions is located in the file Reaction.Lib, (in process of being created).

Variable	Data Type or (Units)	Default Value	Description
RXName	character	none	Is the array of reaction index number, i.e. f1, f2, etc., and a representation of the chemical reaction.
RCInit	(1/second)	none	Is the rate constant for the chemical reaction at the reference temperature.
EA	(kJ/mole K)	none	Is the activation energy for the chemical reaction.

A partial example of this input section is shown below, for the full set view the sample input file attached in the next section:

```
$Reaction
 f3   e-   H2O    >H    OH-        1.6e1      12.55
 f4   e-   H+     >H               3.5e+11     0.e0
 f5   e-   OH     >OH-             2.0e+10    12.55
 f6   e-   H2O2   >OH    OH-       1.3e+11     0.e0
 f7   H    H      >H2              8.5e10      0.e0
$End OF REACTION
```

Group Name: Component

This group describes the system configuration and is generated by drawing a schematic of the system including all components in parallel or series and the nodes at which these components join. These parameters are read line by line, therefore all data pertaining to a reaction set must be contained on one line.

Variable	Data Type or (Units)	Default Value	Description
CompName	Character	none	Is the component name.
CompNode	integer	none	Is an array containing the input and output nodes of a component.

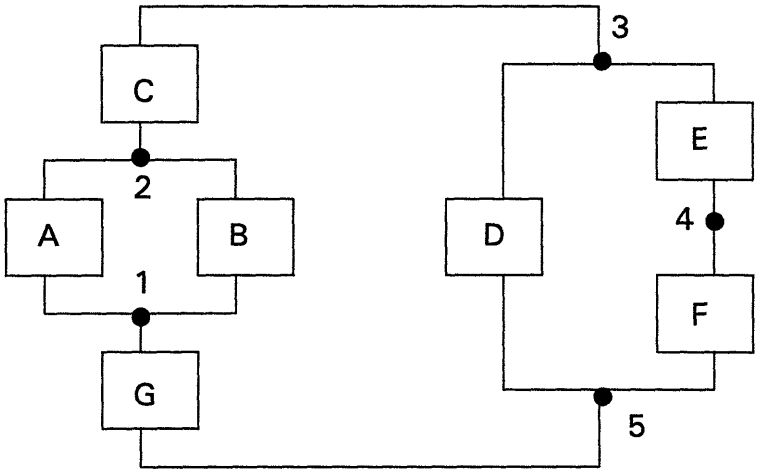

Figure A.1 Sample System Schematic.

A sample input for the configuration shown in Fig. A.1 is given below:

```
$Component
A     1  2
B     1  2
C     2  3
D     3  5
E     3  4
F     4  5
G     5  1
$End
```

Component Parameters

Group Name: Position

This group specifies the axial location of components, phenomena, and output locations.

Variable	Data Type or (Units)	Default Value	Description
Xin	(cm)	0 - 1st comp	Is the initial position of the of the channel along a flow path consisting of all the components. This is set to zero for the first component. XIn for Subsequent components are .calculated automatically by adding the variable XLength to determine an XOut. This XOut is the next components XIn.
XLength	(cm)	1.d0	Is the nominal length of the component.
XStep	(cm)	0.d0, component midpoint and endpoint.	Is the position at which data is written to the output file. If other locations are desired they must be specified.
XBoil	(cm)	9999.d0	Is the position for onset of boiling in two phase flow regions. This is calculated automatically for the Chexal model, however it must be specified for the Bankoff model
XBoilOffset	(cm)	1.d-10	If XBoil = XLength a divide by zero error will occur. To avoid this variable is subtracted from XLength.
PlotStep	(cm)	0.d0, 10 equally spaced intervals, and endpoint.	Is the position at which data is written to the plot file. The default positions are at the inlet, outlet and ten equally spaced intervals for each component. If other locations are desired they must be specified.

Group Name: State

This group identifies thermalhydraulic properties of the component.

Variable	Data Type or (Units)	Default Value	Description
TempIn	(Kelvin)	0.d0	Is the temperature at the component inlet in Kelvin. This is normally specified for the first component. The values for subsequent components are calculated using the heat balance routine. The given values are typically the core inlet temperatures and the feedwater inlet temperature. These are obtained from the plant operational data. If the heat balance is not calculated then all components must have this value declared.
TempOut	(Kelvin)	298.0	Is normally calculated using the heat balance for all components. If the heat balance is not calculated then all components must have this value declared.
Pressure	(MPa)	1.d0	Is the operating pressure of the primary system in MPa. It is specified for the first component and all subsequent components default to this value. This is obtained from plant operational data.
Diameter	(cm)	0.d0	is the hydraulic diameter of the component in cm. If it is not declared the diameter is calculated from the area assuming a circular pipe. This value can be calculated from plant data.
FlowRate	(g/sec)	0.d0	Is the mass flow rate in grams per second. This value is normally calculated from the total flow rate and the flow fraction in the program. It can be obtained from plant operational data
FlowFrac	(%/100)	none	Is the fraction of the total flow through the component. This is set at 1 unless there are components in parallel and components where a portion of the flow is diverted to the steam turbines It must be declared in the input file.
Surface	character	blank	is the surface material of the component

AreaIn	(cm^2)	0.d0	is the cross-sectional area of the component at the inlet in cm^2.
AreaOut	(cm^2)	0.d0	is the cross-sectional area of the component at the outlet in cm^2.
CarryUnder		0.d0	is the mass fraction of steam. This is used to determine component inlet enthalpy if heat balance calculations are not done.
CarryOver		0.d0	is the mass fraction of liquid. This is used to determine component inlet enthalpy if heat balance calculations are not done.
QualMin		1.d-5	is the minimum quality under which the fluid is considered to be single-phase.
Diffusion		3.5d-4	is the diffusion rate of chemical species through the fluid. This is used in considering surface decomposition effects.
Viscosity		1.4d-3	is the viscosity of the fluid. This is also used in considering the surface decomposition effects.
FlowOrient		0.d0	Is the direction of the fluid flow. This is a parameter for the Chexal-Lellouche thermodynamic routines.

Group Name: DoseShape

This group describes the radiation field axially along the components length.

Variable	Data Type or (Units)	Default Value	Description
GammaAvg	(rad/s)	0.d0	Is the average gamma radiation dose rate in the component.
NeutAvg	(rad/s)	0.d0	Is the average neutron radiation dose rate in the component.
GammaInMode	character	polynomial	This is a flag variable which identifies the data being entered as GammaCoef. Options are polynomial or data points.
GammaCoef	real	1.d-99	These are coefficients for a polynomial which describes the intensity of the radiation along the component length.
NeutInMode	character	polynomial	This is a flag variable which identifies the data being entered as NeutCoef. Options are polynomial or data points.

NeutCoef	real	1.d-99	These are coefficients for a polynomial which describes the intensity of the radiation along the component length.

Group Name: PowerShape

This group is required if the FlowModel flag for the component is set as Chexal, the default value. If the flag is set to BankoffVoid or BankoffQual this group can be omitted.

Variable	Data Type or (Units)	Default Value	Description
PowerAvg	(watts)	0.d0	Is the average power level in the reactor core
PowerInMode	character	datapoints	This is a flag variable which identifies the data being entered as GammaCoef. Options are polynomial or data points.
PowerData	(%/100)	none	These data points identify the fraction of power level along the component length. The power is then calculated by interpolating between these points and multiplying by the average power level.

Group Name: VoidCoef

This group is required if the FlowModel flag for the component is set as BankoffVoid. If the flag is set to Chexal or BankoffQual this group can be omitted.

Variable	Data Type or (Units)	Default Value	Description
VoidInMode	character	none	This is a flag variable which identifies the data being entered as VoidCoef. Options are polynomial or data points.
VoidCoef	real	1.d-99	These are coefficients for a polynomial which describes the void fraction of the two-phase flow along the component length.

Group Name: QualShape

This group is required if the FlowModel flag for the component is set as BankoffQual. If the flag is set to Chexal or BankoffVoid this group can be omitted.

Variable	Data Type or (Units)	Default Value	Description
QualInMode	character	none	This is a flag variable which identifies the data being entered as QualCoef. Options are polynomial or data points.
QualCoef	real	none	These are coefficients for a polynomial which describes the quality of the two-phase flow along the component length.

Group Name: InitialConc

This group sets approximate values for chemical species to begin the iterative calculations. These values are only retained for the first cycle, then overwritten by subsequent calculations.

Variable	Data Type or (Units)	Default Value	Description
ConcInit	(ppb)	none	The initial concentrations for each chemical species are declared under this variable. Generally hydrogen, oxygen, and hydrogen peroxide are individual declared, on one line separated by commas. The other species are lumped together by adding 12*0.d0 to the end of the line.

Group Name: Flag

This group specifies the models to be used in calculating concentrations. Also controls output format and sensitivity calculations.

Variable	Data Type or (Units)	Default Value	Description
SurfComp	logical	true	Is a flag used for hydrogen surface decomposition effects. True results in consideration of this surface effect, false neglects it.

FlowModel	character	Chexal	Is a flag which identifies the thermalhydraulic model to use in calculating fluid properties, SinglePhase for one-phase flow. In two-phase regions. the options are Chexal, BanKoffVoid, or BankoffQual.
SensComp	logical	false	Flag used to identify individual components for sensitivity analysis. True calculates sensitivities, false does not. True values are overridden if SensLoop is false.
WriteRX	logical	false	Flag which indicates whether operating temperature chemical reaction rates are to be included in the output file for a component. True writes the reactions, false does not.
WritePara	logical	true	Flag for including operating parameters with each concentration entry in the output files. True writes the parameters, false does not.
RadHeat	logical	false	Flag for considering nuclear heating from gamma and neutron radiation. True calculates this, false does not.
ThermoModel	character	PowerIn	Is a flag specifying what model to use for determining the temperature profile in a component. PowerIn calculates based on a heat balance, TinTout calculates by interpolating between specified inlet and outlet temperatures.

Group Name: Sensitivity

This group sets the parameters for the sensitivity calculations.

Variable	Data Type or (Units)	Default Value	Description
SensStep	(cm)	0	Is the dx value used in the evaluation of sensitivity
SensSpecies	character	blank	Is the name array for chemical species to conduct sensitivities on.

Group Name: LSODEData

This group sets the control parameters for the sensitivity function in the LSODE subroutine. For a complete description see the LSODE subroutine.

Variable	Data Type or (Units)	Default Value	Description
ITask	integer	4	is a flag indicating the task to be performed.
RTol		1.d-5	is the relative tolerance parameter
ITol	integer	1	is a flag to show if Itol is either a scalar (1) or an array (2)
ATol		1.d-15	is the absolute tolerance parameter
ConcRWork		0.d0	is the real work array of length
IWork	integer	0	is the integer work array length
MF	integer	21	is a method flag
IOpt	integer	0	is to indicate if optional inputs are used, zero implies none.
IState	integer	1	Is a flag if LSODE is unsuccessful.

Group Name: AdjData

This group sets the control parameters for the adjoint function in the LSODE subroutine. For a complete description see the LSODE subroutine.

Variable	Data Type or (Units)	Default Value	Description
AdjITask	integer	4	is a flag indicating the task to be performed.
AdjRTol		1.d-4	is the relative tolerance parameter
AdjITol	integer	1	is a flag to show if Itol is either a scalar (1) or an array (2)
AdjATol		1.d-10	is the absolute tolerance parameter
AdjMF		21	is the real work array of length
AdjIOpt	integer	0	is the integer work array length
AdjRWork	integer	0.d0	is a method flag
AdjIWork	integer	0	is to indicate if optional inputs are used, zero implies none.

Group Name: ResData

This group sets the control parameters for the response function in the LSODE subroutine. For a complete description see the LSODE subroutine.

Variable	Data Type or (Units)	Default Value	Description
ResITask	integer	4	is a flag indicating the task to be performed.
ResRTol		1.d-5	is the relative tolerance parameter
ResITol	integer	0	is a flag to show if Itol is either a scalar (1) or an array (2)

ResATol		1.d-15	is the absolute tolerance parameter
ResMF		21	is the real work array of length
ResIOpt	integer	1	is the integer work array length
ResRWork	integer	0.d0	is a method flag
ResIWork	integer	0	is to indicate if optional inputs are used, zero implies none.

3. Input File Parameter Requirements

Incorporation of variables depends heavily on the choices made for thermalhydraulic model use and flag specifications. In an attempt to ease input file creation a listing of groups and parameters needed for each of these choices will be outlined below. This may not be a complete list as modifications in the program may add or subtract from this list. First the standard operating case will be outlined, then each flag will be discussed with any required changes.

The parameters having default values which do not need to be changed in most cases, unless special cases are desired. This list does not include flags, changes in which will be described later.

Loop					
FileName	**Control**	**Component**	**GValue**	**RXControl**	**Reaction**
	NodeStart			TempRef	
	Debug			WaterImplicit	
	CalcConc				
	CycleOut				
	CyclePlot				
	ConcInMode				
	ConcOutMode				
	ConvMin				

Component					
Position	**State**	**DoseShape**	**PowerShape**	**VoidCoef**	**QualShape**
XIn	QualMin	GammaInMode	PowerInMode	VoidInMode	QualInMode
XStep	Diffusion	NeutInMode			
XBoilOffset	Viscosity				
PlotStep	FlowOrient				

InitialConc	**Flag**	**Sensitivity**	**LSODEData**	**AdjData**	**ResData**
	WriteRX		ITask	AdjITask	ResITask
	WritePara		RTol	AdjRTol	ResRTol
	RadHeat		ITol	AdjITol	ResITol
			ATol	AdjATol	ResATol

ConcRWork	AdjMF	ResMF
IWork	AdjIOpt	ResIOpt
MF	AdjRWork	ResRWork
IOpt	AdjIWork	ResIWork
IState		

The groups and parameters which must be included in the input file for the standard radical run are:

Loop					
FileName	**Control**	**Component**	**GValue**	**RXControl**	**Reaction**
OutFile	NCycle	CompName	SpeciesName	NSurfRX	RXName
PlotFile	FlowRateTot	CompNode	GGamma		RCInit
	HeatBalComp		GNeut		EA
			MolWt		

Component					
Position	**State**	**DoseShape**	**PowerShape**	**InitialConc**	**Flag**
XLength	TempIn*	GammaAvg+	PowerAvg+	ConcInit*	
	Pressure**	NeutAvg+	PowerData+		
	Diameter	GammaCoef+			
	FlowFrac	NeutCoef+			
	AreaIn				
	AreaOut++				

* Required for the first node only
** Required for the first component only
\+ Needed only for components where phenomena occurs
++ Needed if variable cross-sectional area component.

Next the effect changes in the default value of flags will have on the standard input file will be identified.

FLAG	**Old Value\ NewValue**	**Changes** Parameter changes unless otherwise noted
Loop		.
PlotOut	true/false	PlotFile can be omitted.
SensLoop	false/true	This must be in conjunction with SensComp and will be discussed in detail there.
HeatBalance	true/false	TempIn, TempOut, CarryUnder, CarryOver, XBoil, must be included. BankoffVoid or BankoffQual must be used for two-phase FlowModel.
ConvComp	blank/ Component name	NCycle can be omitted. ConvComp and ConvSpecies must be included.
InjectHWC	false\true	InjectFile, InjectComp, InjectSpecies, and Inject must be included.
Component		Applicable for each individual component this occurs in.

SensComp	false/true	If this is true and SensLoop is true, The groups Sensitivity, LSODEData, AdjData, and ResData must be included. SensStep, and SensSpecies must be included.
FlowModel	Chexal\	Group PowerShape can be omitted.
	BankoffVoid	Group VoidCoef must be included. VoidCoef must be included
	Chexal\	Group PowerShape can be omitted.
	BankoffQual	Group QualShape must be included. QualCoef must be included.
	Chexal\	Group PowerShape can be omitted.
	SinglePhase	
ThermoModel	PowerIn/	TempIn must be included.
	TinTout	TempOut must be included.
FlowFrac		If not included, FlowRateTot can be omitted FlowRate must be included.

4. Calculation of Parameters

This section describes the calculation or acquisition of physical parameters. The majority of the discussion will regard calculation of BWR primary coolant flow geometry other parameters will be briefly discussed as to their source.

Power profiles, total flow, flow fractions, operating pressures, operating temperatures, void fraction profile, and quality profile can be calculated using thermal-hydraulic computer codes developed to aid in design of theses reactor systems. These values, excluding the profiles, are typically given in the facility safety analysis reports (SAR), however values from the SAR are generally for the design basis operating case used for accident analysis and generally not the actual operating condition.

Dose values can be calculated approximately in the core using neutron theory, with these base values used to determine dose in other areas using shielding

theory for attenuation. Another method would be to use computer codes to determine the doses analytically.

For determining flow geometry two methods are considered, the first is the method used for the simulations in this report where parameters were calculated from residence times obtained from the EPRI report authored by GE [1995]. The second is methods discussed to calculate parameters from plant drawings and data.

Data obtained from the EPRI report consisted primarily of mass flow rates, residence times, and length for each component. From these it is possible to estimate the region cross-sectional area using the following relationship.

$$\dot{m} = \frac{AL\rho}{t} \tag{A.1}$$

where:
m: is the mass flow rate
A: is the cross-sectional area
L: is the component length
t : is the residence time
ρ: is the average fluid density in the component

The hydraulic diameter is calculated using the equation

$$D = \frac{4A}{P_w} \tag{A.2}$$

where:
D: is the hydraulic diameter
Pw: is the wetted perimeter

This equation gives the normal diameter for traditional pipes and the gap between pipe surfaces for annular flow. The hydraulic diameter calculated using this method is only valid for turbulent flow regime such as that found in BWR

under normal operating conditions, but may not be valid at points during start-up and shut-down. To determine the wetted perimeter all surfaces in contact with the fluid should be incorporated not just the surfaces containing the flow. Examples are:

Lower Downcomer: shroud wall, pressure vessel wall, and jet pump walls

Core Boiling: fuel rods and the stainless steel channel skirting

Lower Plenum: pressure vessel walls and control rod drive tube walls.

These parameters for radially segmented regions such as the downcomer were calculated by determining the whole region area, as described above, and fractional component areas using simplified annular geometry with equal width subdivisions. The area fractions calculated for the five regions were then multiplied by the total area and mass flow rate. Dose rates were calculated using shielding theory at the radii used to determine the fractional areas. Hydraulic diameters for these regions are assumed to be the same as for the larger region.

To determine these parameters from plant drawings the residence time must first be determined. Although the dimensions may be accurately characterized using computerized, the geometry so defined may not accurately describe the fluid flow path. This especially true in regions where the flow is not axial such as the bottom of downcomers and the lower plenum. Residence time can be calculated using the following equation, a variation of Eq. A.1:

$$t = \frac{V\rho}{\dot{m}} \qquad \text{(A.3)}$$

Here the component volume (V) is used instead of the area and length. The volume and average component area should then be calculated and inserted into Eq. A.1 to calculated an effective component length. Variable cross-sectional areas and hydraulic diameters can be calculated at intervals along this length, with any values located beyond the effective length neglected. While this may still not be completely accurate, if the parameters are determined from computerized drawings it may be the highest accuracy available with the current one dimensional model.

Appendix B Sample Input File

The input file used for the typical BWR-3 is listed in this appendix as a sample. This file has been altered to exclude any proprietary data obtained from EPRI report TR-106068 [Romeo 1995]. The format can be utilized for any BWR configuration containing jet pumps, with the only difference the values for the input parameter values. This sample file can also serve as a starting point for other BWR system configurations.

1. BWR-3 Input File

```
BWR3.IN is modified from the standrard MIT BWR model developed during
 the 1995 to 1996 Academic Year
 modified for RADICAL version 1.6b25 on 7/10/96

 GE H2O2 decomp rates used
 * 1990 GE reaction rates and G-values used
 * Ibe's mass transfer coefficients are used
 * H2O2 thermal decomposition has been added through W32
 * 1995 GE Surface decomposition rate is fixed at 280C  througsh SS

 &FileName
 OutFile  = 'c:\radical\data\bwr3\bwr3.OUT'
 PlotFile = 'c:\radical\data\bwr3\bwr3.PLO'
 InjectFile  = 'c:\radical\data\bwr3\bwr3.HWC' /

 &Control
 FlowRateTot = 8.5e6
 HeatBalComp = 'PRE MIXING'
 ConvComp    = 'CORE BOILING'
 ConvSpecies = 'H2','O2','H2O2'
 CalcInject  = t
 InjectComp  = 'FEEDWATER'
 Inject      = 0.0,90.0,160.0,240.0,360.0,530.0,710.0,870.0,1000.0,
           1130.0,1240.0,1360.0,1450.0,1960.0,2500.0 /

*1234567890123456+123+123

 $Component
 CORE BOILING              1   2
 CORE BYPASS               1   2
```

```
OUTER BYPASS          1   2
UPPER PLENUM          2  15
SEPARATOR 2PHASE     15  16
SEPARATOR 1PHASE     16  17
PRE MIXING           17   3
FEEDWATER            14   3
MIXING PLENUM         3   4
UP DOWNCOMER A        4   5
UP DOWNCOMER B        4   5
UP DOWNCOMER C        4   5
UP DOWNCOMER D        4   5
UP DOWNCOMER E        4   5
LO DOWNCOMER A        5   6
LO DOWNCOMER B        5   6
LO DOWNCOMER C        5   6
LO DOWNCOMER D        5   6
LO DOWNCOMER E        5   6
JET PUMP SUCTION      5  10
SAMPLE                6  10
RECIRC OUTLET         6   7
RECIRC MANIFOLD       7   8
RECIRC INLET          8   9
JET PUMP RISER        9  10
JET PUMP THROAT      10  18
JET PUMP DIFFUSE     18  19
JET PUMP TAIL        19  11
LOWER PLENUM         11  12
CORE PLATE           12   1
$End

**********8**********************************************************************
GE.DAT                          Wednesday, July 28, 1993 2:40:16 PM
LAST MODIFIED: Wednesday, July 28, 1993 2:40:16 PM
*from GE report "Radiolysis Code" presented by Carl Ruiz,
Aug 1992 at MIT
*GE's Hi-T Gamma G-VALUES (1992)
*GE's Hi-T Neutron G-VALUES (1992)

Abcdefgh+12345678901234+12345678901234+12345678901234

$GValue
H2          0.80              0.88              2.000D+00
O2                                              3.200D+01
H2O2        0.28              0.99              3.400D+01
O2G                                             3.200D+01
H2G                                             2.000D+00
```

H+	3.7600	0.93	1.000D+00
OH-			1.700D+01
e-	3.7600	0.93	5.490D-04
OH	5.500	1.09	1.700D+01
HO2-			3.300D+01
O2-			3.200D+01
H	0.700	0.5	1.000D+00
HO2		0.04	3.300D+01
1/2O2			16.0
H2O			18.0

$End OF GValue

*REACTION NAME, REACTION, RATE CONSTANT AND ACTIVATION ENERGY
WATER EXPLICITLY DECLARED
&RxControl
NSurfRx = 1/

Abc AbcdefghAbcdefghAbcdefgh AbcdefghAbcdefghAbcdefghAbcdefgh+12345678901234+12345678901234

$Reaction

f3	e-	H2O	>H	OH-		1.6e1	12.55
f4	e-	H+	>H			3.5e+11	0.e0
f5	e-	OH	>OH-			2.0e+10	12.55
f6	e-	H2O2	>OH	OH-		1.3e+11	0.e0
f7	H	H	>H2			8.5e10	0.e0
f8	e-	HO2	>HO2-			2.0e10	12.55
f9	e-	O2	>O2-			2.6e11	0.e0
f10	e-	e-	>OH-	OH-	H2	5.e9	12.55
f11	OH	OH	>H2O2			1.7e10	0.e0
f12	H	OH-	>e-	H2O		2.0e7	18.83
f13	H	e-	>H2	OH-		2.5e10	12.55
f14	HO2-	e-	>OH	OH-	OH-	3.5e9	12.55
f15	H	OH	>H2O			5.5e10	0.e0
f16	H2	OH	>H	H2O		4.e7	18.0163
r16	H	H2O	>OH	H2		1.042e-4	85.1695
f17	H	O2	>HO2			8.6e10	0.e0
f18	H	HO2	>H2O2			2.e10	12.55
f19	H	O2-	>HO2-			2.e10	12.55
f20	O2-	e-	>HO2-	OH-		1.3e8	18.83
f21	H	H2O2	>OH	H2O		9.e7	16.61466
f22	H2O2	OH	>H2O	HO2		3.e7	13.01224
f23	HO2	OH	>O2	H2O		8.6e10	0.e0
f24	H2O2	OH-	>HO2-	H2O		1.8e10	12.55
r24	HO2-		>H2O2	OH-		5.7e5	18.83

```
f25   HO2  HO2        >O2     H2O2    8.5e5          22.82372
f26   HO2             >H+     O2-     2.565e4        12.55
r26   O2-  H+         >HO2            5.e10          12.55
f27   HO2  O2-        >HO2-   O2      5.e9            0.e0
f29   H+   OH-        >H2O            1.44e11        12.55
r29                   >H+     OH-     0.7924273190   12.55
f30   OH   O2-        >O2     OH-     8.6e10          0.e0
tif 1 /2O2 1/2O2      >O2             1.e15           0.e0
W32   H2O2            >OH     OH      2.00E-03        0.0
h2g   H2              >H2G            30.            -1.0
h2l   H2G             >H2             10.            -1.0
o2g   O2              >O2G            23.            -1.0
o2l   O2G             >O2             12.            -1.0
SS    H2O2            >1/2O2  H2O     0.124           0.0
$End OF REACTION

**********************************************************************
@CORE BOILING

&Position
XLength  = 366.0 /

&State
TempIn   = 549.5
Pressure = 7.2
FlowFrac = 0.89
Diameter = 1.3
AreaIn   = 6.7033d4 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1.e5
GammaCoef= 0.1780,0.8231,1.2013,1.3347,1.4015,1.4237,1.4237,
        1.4237,1.4237,1.4237,1.3792,1.3792,1.3125,1.1790,
        1.0011,0.7341,0.3337,0.1335
NeutAvg  = 2.77e5
NeutCoef = 0.1477,0.6571,0.9483,1.0689,1.1653,1.2457,1.3020,
        1.3582,1.4145,1.4707,1.4948,1.5189,1.5350,1.5029,
        1.4064,1.2216,0.9162,0.4259,0.1286 /

&PowerShape
PowerAvg = 1.998d9
PowerData= 0.0,0.26257,0.94197,1.23177,1.34951,1.35377,1.35793,
        1.31032,1.26297,1.22539,1.18018,1.14267,1.11292,
        1.09086,1.07348,1.07312,1.05093,1.00495,0.97469,
```

```
        0.93813,0.91278,0.8257,0.69042,0.45963,0.17333 /

&InitialConc
ConcInit = 22.0,0.06,4.0,12*0.0, /

&Flag/
&Sensitivity /
&LSODEData /

@End OF CORE BOILING
*********************************************************************
@CORE BYPASS

&Position
XLength  = 366.0 /

&State
TempIn   = 549.5
FlowFrac = 0.10
AreaIn   = 5.3210d4
Diameter = 4.27 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 6.33E4
GammaCoef= 0.1564,0.8893,1.2066,1.3184,1.3854,1.4077,1.4077,
        1.4301,1.4077,1.4077,1.3854,1.3631,1.2960,1.1843,
        1.0055,0.7597,0.3352,0.1341
NeutAvg  = 2.77e5
NeutCoef = 0.1477,0.6571,0.9483,1.0689,1.1653,1.2457,1.3020,
        1.3582,1.4145,1.4707,1.4948,1.5189,1.5350,1.5029,
        1.4064,1.2216,0.9162,0.4259,0.1286 /

&VoidShape /
&PowerShape /

&InitialConc
ConcInit = 22.0,0.06,4.0,12*0.0, /

&Flag /
&Sensitivity /
&LSODEData /

@End OF CORE BYPASS
*********************************************************************
```

```
@OUTER BYPASS

&Position
XLength  = 366.0 /

&State
TempIn   = 549.5
FlowFrac = 0.01
AreaIn   = 1.064d3
Diameter = 5.0 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1.2150E4
GammaCoef= 0.1564,0.8893,1.2066,1.3184,1.3854,1.4077,1.4077,
        1.4301,1.4077,1.4077,1.3854,1.3631,1.2960,1.1843,
        1.0055,0.7597,0.3352,0.1341
NeutAvg  = 4.500e3
NeutCoef = 0.1477,0.6571,0.9483,1.0689,1.1653,1.2457,1.3020,
        1.3582,1.4145,1.4707,1.4948,1.5189,1.5350,1.5029,
        1.4064,1.2216,0.9162,0.4259,0.1286 /

&VoidShape /
&PowerShape /

&InitialConc
ConcInit = 22.0,0.06,4.0,12*0.0, /

&Flag /
&Sensitivity /
&LSODEData /

@End OF OUTER BYPASS
**********************************************************************
@UPPER PLENUM

&Position
XLength  = 175.8 /

&State
FlowFrac =  1.0
AreaIn   =  1.9722d5
Diameter =  501.0 /

&DoseShape
```

```
GammaInMode=1
NeutInMode =1
GammaAvg = 878.0
GammaCoef= 15.2022,5.0674,4.3861,3.3228,2.6804,2.1266,
        1.7278,1.3734,1.1076,0.8861,0.7089,0.5759,
        0.4652,0.3766,0.2880,0.2437,0.1994,0.1551,
        0.1108,0.0886,0.0665,0.0665,0.0443
NeutAvg =  427.0
NeutCoef=  88.6303,10.4267,7.1487,4.6899,3.1418,2.0490,
         1.3205,0.8651,0.5919,0.4098,0.2732,0.1821,
         0.1366,0.0911,0.0455,0.0455,0.0091,0.0,
         0.0,0.0,0.0,0.0,0.0 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF UPPER PLENUM
**********************************************************************
@SEPARATOR 2PHASE

&Position
XLength  = 260.7 /

&State
FlowFrac = 1.0
AreaIn   = 34249.2
Diameter = 15.4 /

&DoseShape
GammaAvg = 20.0
GammaCoef= 1.0 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF SEPARATOR 2PHASE
**********************************************************************
@SEPARATOR 1PHASE

&Position
```

```
XLength  = 115.54 /

&State
TempIn  = 559.0
FlowFrac = 0.885
AreaIn   = 16396.75
Diameter = 4.0 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag  /
&Sensitivity /
&LSODEData /

@End OF SEPARATOR 1PHASE
**********************************************************************
@FEEDWATER

&Position
XLength  = 0.1
XStep    = 0.1 /

&State
TempIn   = 444.3
FlowFrac = 0.115
Diameter = 27.31
AreaIn   = 3513.6 /

&InitialConc /
&DoseShape /
&VoidShape /
&Flag /
&Sensitivity /
&LSODEData /

@End OF FEEDWATER
**********************************************************************
@PRE MIXING

&Position
XLength  = 119.0 /

&State
TempIn = 559.0
FlowFrac = 0.885
```

```
AreaIn   = 1.91281d5
Diameter = 22.9 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF PRE MIXING
**********************************************************************
@MIXING PLENUM

&Position
XLength  = 118.9 /

&State
FlowFrac = 1.0
AreaIn   = 1.91281d5
Diameter = 22.9 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF MIXING PLENUM
**********************************************************************
@UP DOWNCOMER A

&Position
XLength  = 298.0 /

&State
FlowFrac = 0.184
AreaIn   = 5111.0
Diameter = 63.6 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 3184.2
GammaCoef= 0.0,0.0030,0.0304,0.1216,0.3953,1.06414,
```

```
        1.8698,2.4323,2.5691
NeutAvg  = 6941.0
NeutCoef = 0.0,0.00505,0.0252,0.0505,0.2523,1.0344,
        2.0435,2.5228,2.6490 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF UP DOWNCOMER A
*****************************************************************
@UP DOWNCOMER B

&Position
XLength  = 298.0 /

&State
FlowFrac = 0.192
AreaIn   = 5333.2
Diameter = 63.6 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 2415.6
GammaCoef= 0.0,0.0030,0.0304,0.1216,0.3953,1.06414,
        1.8698,2.4323,2.5691
NeutAvg  = 2761.0
NeutCoef = 0.0,0.00505,0.0252,0.0505,0.2523,1.0344,
        2.0435,2.5228,2.6490 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF UP DOWNCOMER B
*****************************************************************
@UP DOWNCOMER C

&Position
XLength  = 298.0 /
```

```
&State
FlowFrac = 0.2
AreaIn   = 5555.54
Diameter = 63.6 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1830.0
GammaCoef= 0.0,0.0030,0.0304,0.1216,0.3953,1.06414,
        1.8698,2.4323,2.5691
NeutAvg  = 1100.0
NeutCoef = 0.0,0.00505,0.0252,0.0505,0.2523,1.0344,
        2.0435,2.5228,2.6490 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF UP DOWNCOMER C
**********************************************************************
@UP DOWNCOMER D

&Position
XLength  = 298.0 /

&State
FlowFrac = 0.208
AreaIn   = 5777.6
Diameter = 63.6 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1390.8
GammaCoef= 0.0,0.0030,0.0304,0.1216,0.3953,1.06414,
        1.8698,2.4323,2.5691
NeutAvg  = 437.8
NeutCoef = 0.0,0.00505,0.0252,0.0505,0.2523,1.0344,
        2.0435,2.5228,2.6490 /

&VoidShape /
&InitialConc /
&Flag /
```

```
&Sensitivity /
&LSODEData /

@End OF UP DOWNCOMER D
*********************************************************************
@UP DOWNCOMER E

&Position
XLength  = 298.0 /

&State
FlowFrac = 0.216
AreaIn   = 5999.8
Diameter = 63.6 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1052.25
GammaCoef= 0.0,0.0030,0.0304,0.1216,0.3953,1.06414,
        1.8698,2.4323,2.5691
NeutAvg  = 173.8
NeutCoef = 0.0,0.00505,0.0252,0.0505,0.2523,1.0344,
        2.0435,2.5228,2.6490 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF UP DOWNCOMER E
*********************************************************************
@JET PUMP SUCTION

&Position
XLength  = 0.1 /

&State
AreaIn   = 0.1
FlowFrac = 0.500 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
```

```
&Sensitivity /
&LSODEData /

@End OF JET PUMP SUCTION
**********************************************************************
@LO DOWNCOMER A

&Position
XLength  = 495.1 /

&State
FlowFrac = 0.1324
AreaIn   = 17035.9
Diameter = 36.5 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 3184.2
GammaCoef= 2.5691,2.70595,2.7972,2.6147,2.3411,1.5202,
        0.4713,0.0608,0.00304,0.0,0.0,0.0,0.0
NeutAvg  = 6941.0
NeutCoef = 2.6490,2.8256,2.7751,2.5228,2.321,1.4632,
        0.4541,0.0505,0.0050,0.0,0.0,0.0,0.0 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF LO DOWNCOMER A
**********************************************************************
@LO DOWNCOMER B

&Position
XLength  = 495.1 /

&State
FlowFrac = 0.0823
AreaIn   = 10591.6
Diameter = 36.5 /

&DoseShape
GammaInMode=1
NeutInMode =1
```

```
GammaAvg = 2415.6
GammaCoef= 2.5691,2.70595,2.7972,2.6147,2.3411,1.5202,
        0.4713,0.0608,0.00304,0.0,0.0,0.0,0.0
NeutAvg  = 2761.0
NeutCoef = 2.6490,2.8256,2.7751,2.5228,2.321,1.4632,
        0.4541,0.0505,0.0050,0.0,0.0,0.0,0.0 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF LO DOWNCOMER B
**********************************************************************
@LO DOWNCOMER C

&Position
XLength  = 495.1 /

&State
FlowFrac = 0.03224
AreaIn   = 4147.3
Diameter = 36.5 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1830.0
GammaCoef= 2.5691,2.70595,2.7972,2.6147,2.3411,1.5202,
        0.4713,0.0608,0.00304,0.0,0.0,0.0,0.0
NeutAvg  = 1100.0
NeutCoef = 2.6490,2.8256,2.7751,2.5228,2.321,1.4632,
        0.4541,0.0505,0.0050,0.0,0.0,0.0,0.0 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF LO DOWNCOMER C
**********************************************************************
@LO DOWNCOMER D

&Position
```

```
XLength  = 495.1 /

&State
FlowFrac = 0.093744
AreaIn   = 12059.1
Diameter = 36.5 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1390.8
GammaCoef= 2.5691,2.70595,2.7972,2.6147,2.3411,1.5202,
        0.4713,0.0608,0.00304,0.0,0.0,0.0,0.0
NeutAvg  = 437.8
NeutCoef = 2.6490,2.8256,2.7751,2.5228,2.321,1.4632,
        0.4541,0.0505,0.0050,0.0,0.0,0.0,0.0 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF LO DOWNCOMER D
*********************************************************************
@LO DOWNCOMER E

&Position
XLength  = 495.1 /

&State
FlowFrac = 0.1552
AreaIn   = 19971.0
Diameter = 36.5 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1052.25
GammaCoef= 2.5691,2.70595,2.7972,2.6147,2.3411,1.5202,
        0.4713,0.0608,0.00304,0.0,0.0,0.0,0.0
NeutAvg  = 173.8
NeutCoef = 2.6490,2.8256,2.7751,2.5228,2.321,1.4632,
        0.4541,0.0505,0.0050,0.0,0.0,0.0,0.0 /

&VoidShape /
```

```
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF LO DOWNCOMER E
*********************************************************************
@SAMPLE

&Position
XLength  = 2000.0 /

&State
FlowFrac = 1.D-6
AreaIn   = 1.0
Diameter = 0.75 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF SAMPLE
*********************************************************************
@RECIRC OUTLET

&Position
XLength  = 3195.9 /

&State
FlowFrac = 0.500
AreaIn   = 7945.2
Diameter = 71.12 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF RECIRC OUTLET
*********************************************************************
@RECIRC MANIFOLD
```

```
&Position
XLength  = 644.8 /

&State
FlowFrac = 0.500
AreaIn   = 4905.0
Diameter = 55.88 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF RECIRC MANIFOLD
**********************************************************************
@RECIRC INLET

&Position
XLength  = 673.0 /

&State
FlowFrac = 0.500
AreaIn   = 7297.0
Diameter = 30.48 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF RECIRC INLET
**********************************************************************
@JET PUMP RISER

&Position
XLength  = 402.7 /

&State
FlowFrac = 0.500
AreaIn   = 7297.0
Diameter = 30.48 /
```

```
&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1750.0
GammaCoef= 0.0025,0.0504,0.2013,0.6039,1.2078,1.7487,
        1.9626,2.0633,2.2017,2.3023,2.2646,2.1891,
        2.1262,2.0758
NeutAvg  = 1140.0
NeutCoef = 0.0039,0.0579,0.1737,0.5596,1.1193,1.6982,
        1.949,2.0263,2.1227,2.2965,2.354,2.2965,
        2.20,2.1421 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF JET PUMP RISER
**********************************************************************
@JET PUMP THROAT

&Position
XLength  = 226.2 /

&State
AreaIn   = 4686.0
Diameter = 17.27
FlowFrac = 1.0 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1750.0
NeutCoef = 2.1421,2.200,2.2965,2.3544,2.2965,2.1227,
        2.0263,1.949,1.6982,1.1193
NeutAvg  = 1140.0
GammaCoef= 2.0758,2.1262,2.1891,2.2646,2.3023,2.2017,
        2.0633,1.9626,1.7487,1.2078 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /
```

```
@End OF JET PUMP THROAT
**********************************************************************
@JET PUMP DIFFUSE

&Position
XLength  = 152.1 /

&State
AreaIn   = 4686.0
AreaOut  = 28432.6
FlowFrac = 1.0 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 1750.0
NeutCoef = 1.1193,0.5596,0.1737,0.0579,0.0039,0.0,0.0
NeutAvg  = 1140.0
GammaCoef= 1.2078,0.6309,0.2013,0.0504,0.0025,0.0,0.0 /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF JET PUMP DIFFUSE
**********************************************************************
@JET PUMP TAIL

&Position
XLength  = 116.8 /

&State
AreaIn   = 28432.6
Diameter = 42.55
FlowFrac = 1.0 /

&DoseShape /

&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /
```

```
@End OF JET PUMP TAIL
**********************************************************************
@LOWER PLENUM

&Position
XLength  = 536.0 /

&State
AreaIn   = 8.579d4
Diameter = 27.5
FlowFrac = 1.0 /

&DoseShape /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF LOWER PLENUM
**********************************************************************
@CORE PLATE

&Position
XLength  = 16.1 /

&State
AreaIn   = 8.579d4
Diameter = 27.5
FlowFrac = 1.0 /

&DoseShape
GammaInMode=1
NeutInMode =1
GammaAvg = 872.0
GammaCoef= 0.0505,1.2620,19.6875
NeutAvg  = 2290.0
NeutCoef = 0.01925,1.8286,19.1522 /
&VoidShape /
&InitialConc /
&Flag /
&Sensitivity /
&LSODEData /

@End OF CORE PLATE
```